



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:57 AM UTC

PDB ID : 4KK1 / pdb_00004kk1
Title : Crystal Structure of TSC1 core domain from *S. pombe*
Authors : Sun, W.; Zhu, Y.; Wang, Z.Z.; Zhong, Q.; Gao, F.; Lou, J.Z.; Gong, W.M.;
Xu, W.Q.
Deposited on : 2013-05-05
Resolution : 3.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

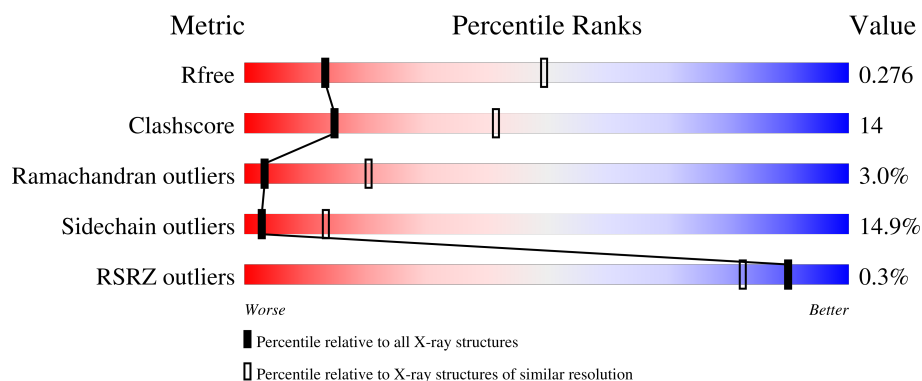
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	434	50% 34% 8% 7%
1	B	434	52% 32% 5% 10%
1	C	434	56% 28% 6% 10%
1	D	434	55% 29% 6% 10%
1	E	434	51% 31% 7% 10%

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Mol	Chain	Length	Quality of chain
1	F	434	
1	G	434	
1	H	434	
1	I	434	
1	J	434	
1	K	434	
1	L	434	
1	M	434	
1	N	434	
1	O	434	
1	P	434	
1	Q	434	
1	R	434	
1	S	434	
1	T	434	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 63794 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Tuberous sclerosis 1 protein homolog.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	403	Total	C	N	O	S	Se	0	0	0
			3268	2116	548	591	8	5			
1	B	391	Total	C	N	O	S	Se	0	0	0
			3181	2066	532	570	8	5			
1	C	391	Total	C	N	O	S	Se	0	0	0
			3181	2066	532	570	8	5			
1	D	391	Total	C	N	O	S	Se	0	0	0
			3181	2066	532	570	8	5			
1	E	391	Total	C	N	O	S	Se	0	0	0
			3181	2066	532	570	8	5			
1	F	391	Total	C	N	O	S	Se	0	0	0
			3181	2066	532	570	8	5			
1	G	391	Total	C	N	O	S	Se	0	0	0
			3181	2066	532	570	8	5			
1	H	391	Total	C	N	O	S	Se	0	0	0
			3181	2066	532	570	8	5			
1	I	391	Total	C	N	O	S	Se	0	0	0
			3181	2066	532	570	8	5			
1	J	391	Total	C	N	O	S	Se	0	0	0
			3181	2066	532	570	8	5			
1	K	403	Total	C	N	O	S	Se	0	0	0
			3268	2116	548	591	8	5			
1	L	391	Total	C	N	O	S	Se	0	0	0
			3181	2066	532	570	8	5			
1	M	391	Total	C	N	O	S	Se	0	0	0
			3181	2066	532	570	8	5			
1	N	391	Total	C	N	O	S	Se	0	0	0
			3181	2066	532	570	8	5			
1	O	391	Total	C	N	O	S	Se	0	0	0
			3181	2066	532	570	8	5			
1	P	391	Total	C	N	O	S	Se	0	0	0
			3181	2066	532	570	8	5			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	Q	391	Total	C	N	O	S	Se	0	0	0
			3181	2066	532	570	8	5			
1	R	391	Total	C	N	O	S	Se	0	0	0
			3181	2066	532	570	8	5			
1	S	391	Total	C	N	O	S	Se	0	0	0
			3181	2066	532	570	8	5			
1	T	391	Total	C	N	O	S	Se	0	0	0
			3181	2066	532	570	8	5			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q09778
A	-1	HIS	-	expression tag	UNP Q09778
A	0	MSE	-	expression tag	UNP Q09778
B	-2	SER	-	expression tag	UNP Q09778
B	-1	HIS	-	expression tag	UNP Q09778
B	0	MSE	-	expression tag	UNP Q09778
C	-2	SER	-	expression tag	UNP Q09778
C	-1	HIS	-	expression tag	UNP Q09778
C	0	MSE	-	expression tag	UNP Q09778
D	-2	SER	-	expression tag	UNP Q09778
D	-1	HIS	-	expression tag	UNP Q09778
D	0	MSE	-	expression tag	UNP Q09778
E	-2	SER	-	expression tag	UNP Q09778
E	-1	HIS	-	expression tag	UNP Q09778
E	0	MSE	-	expression tag	UNP Q09778
F	-2	SER	-	expression tag	UNP Q09778
F	-1	HIS	-	expression tag	UNP Q09778
F	0	MSE	-	expression tag	UNP Q09778
G	-2	SER	-	expression tag	UNP Q09778
G	-1	HIS	-	expression tag	UNP Q09778
G	0	MSE	-	expression tag	UNP Q09778
H	-2	SER	-	expression tag	UNP Q09778
H	-1	HIS	-	expression tag	UNP Q09778
H	0	MSE	-	expression tag	UNP Q09778
I	-2	SER	-	expression tag	UNP Q09778
I	-1	HIS	-	expression tag	UNP Q09778
I	0	MSE	-	expression tag	UNP Q09778
J	-2	SER	-	expression tag	UNP Q09778
J	-1	HIS	-	expression tag	UNP Q09778
J	0	MSE	-	expression tag	UNP Q09778
K	-2	SER	-	expression tag	UNP Q09778

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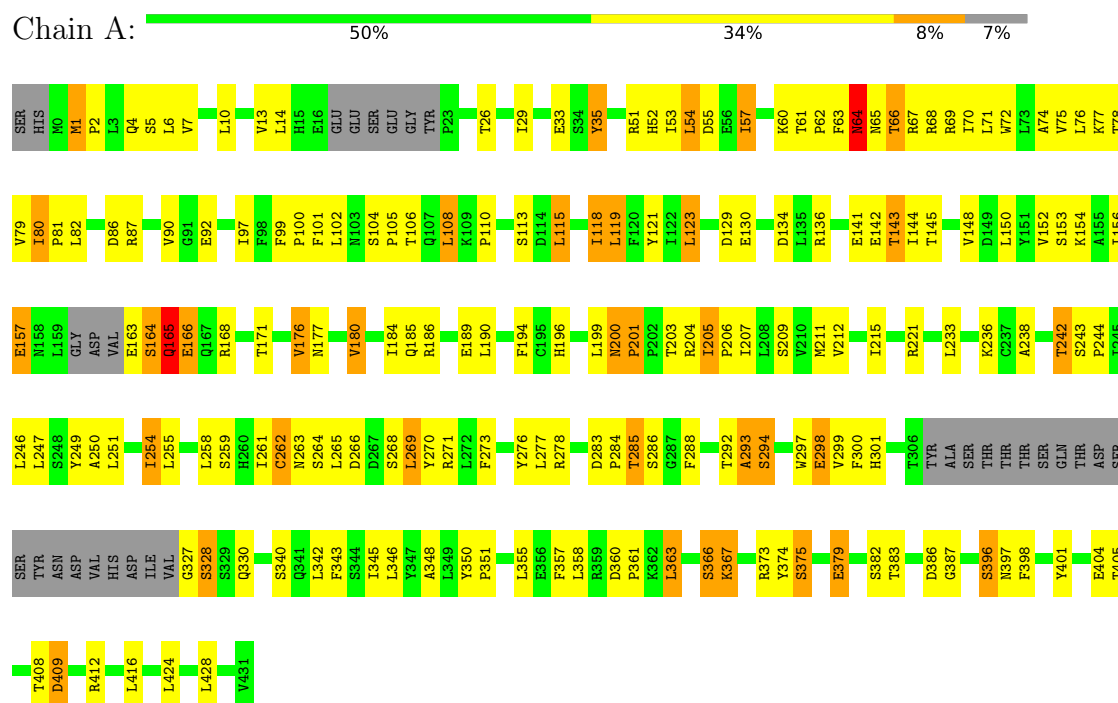
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Chain	Residue	Modelled	Actual	Comment	Reference
K	-1	HIS	-	expression tag	UNP Q09778
K	0	MSE	-	expression tag	UNP Q09778
L	-2	SER	-	expression tag	UNP Q09778
L	-1	HIS	-	expression tag	UNP Q09778
L	0	MSE	-	expression tag	UNP Q09778
M	-2	SER	-	expression tag	UNP Q09778
M	-1	HIS	-	expression tag	UNP Q09778
M	0	MSE	-	expression tag	UNP Q09778
N	-2	SER	-	expression tag	UNP Q09778
N	-1	HIS	-	expression tag	UNP Q09778
N	0	MSE	-	expression tag	UNP Q09778
O	-2	SER	-	expression tag	UNP Q09778
O	-1	HIS	-	expression tag	UNP Q09778
O	0	MSE	-	expression tag	UNP Q09778
P	-2	SER	-	expression tag	UNP Q09778
P	-1	HIS	-	expression tag	UNP Q09778
P	0	MSE	-	expression tag	UNP Q09778
Q	-2	SER	-	expression tag	UNP Q09778
Q	-1	HIS	-	expression tag	UNP Q09778
Q	0	MSE	-	expression tag	UNP Q09778
R	-2	SER	-	expression tag	UNP Q09778
R	-1	HIS	-	expression tag	UNP Q09778
R	0	MSE	-	expression tag	UNP Q09778
S	-2	SER	-	expression tag	UNP Q09778
S	-1	HIS	-	expression tag	UNP Q09778
S	0	MSE	-	expression tag	UNP Q09778
T	-2	SER	-	expression tag	UNP Q09778
T	-1	HIS	-	expression tag	UNP Q09778
T	0	MSE	-	expression tag	UNP Q09778

3 Residue-property plots

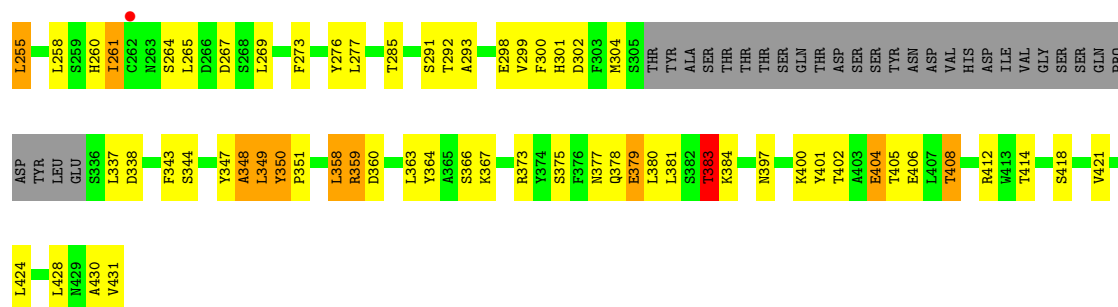
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Tuberous sclerosis 1 protein homolog



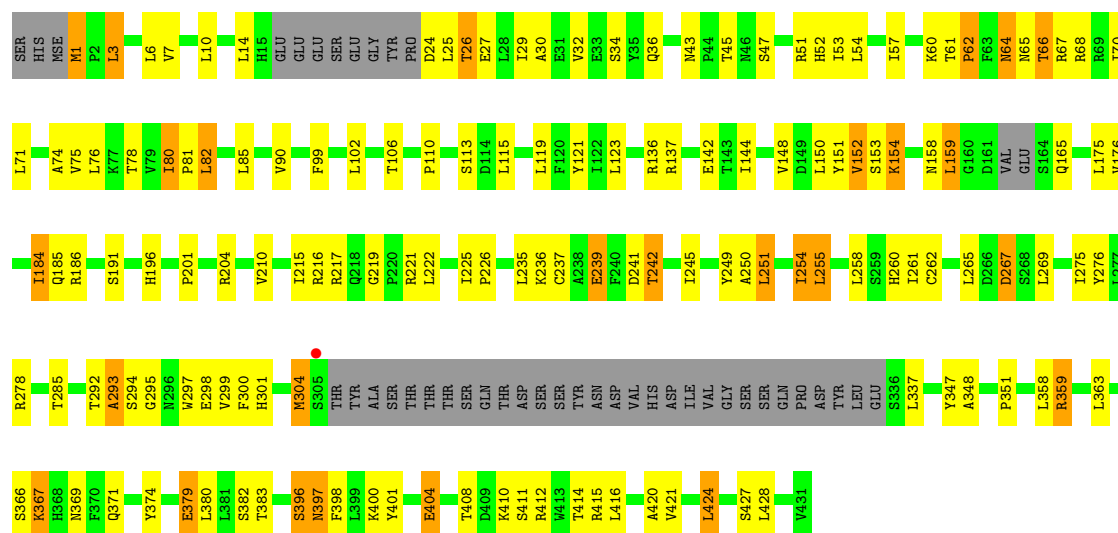
• Molecule 1: Tuberous sclerosis 1 protein homolog





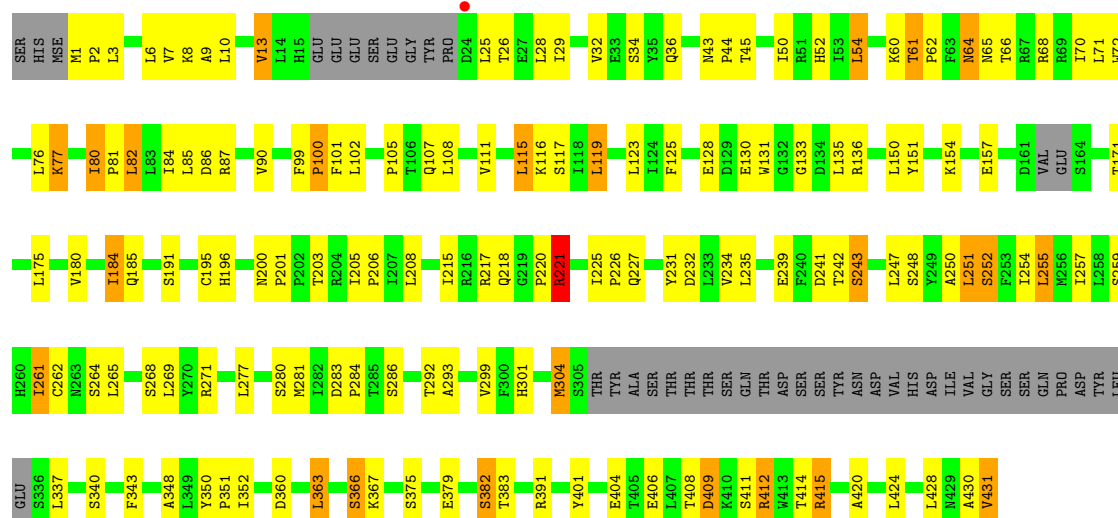
- Molecule 1: Tuberous sclerosis 1 protein homolog

Chain C: 56% 28% 6% 10%



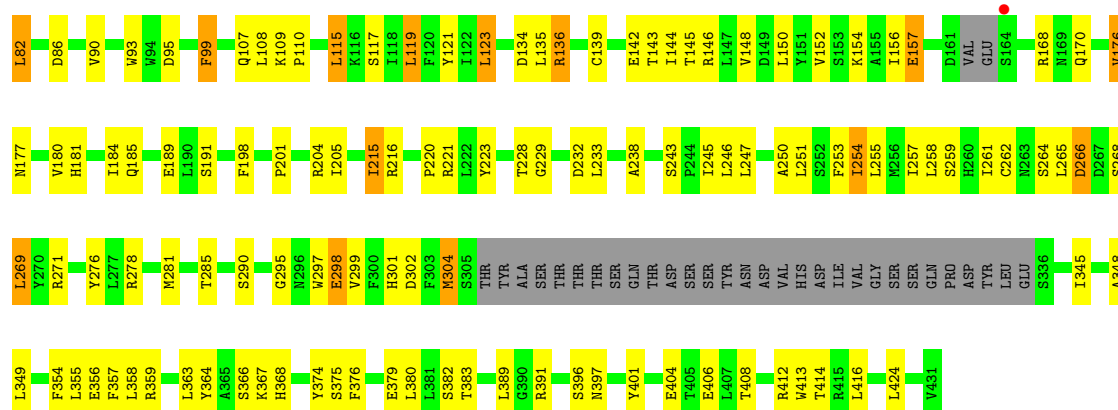
- Molecule 1: Tuberous sclerosis 1 protein homolog

Chain D: 55% 29% 6% 10%



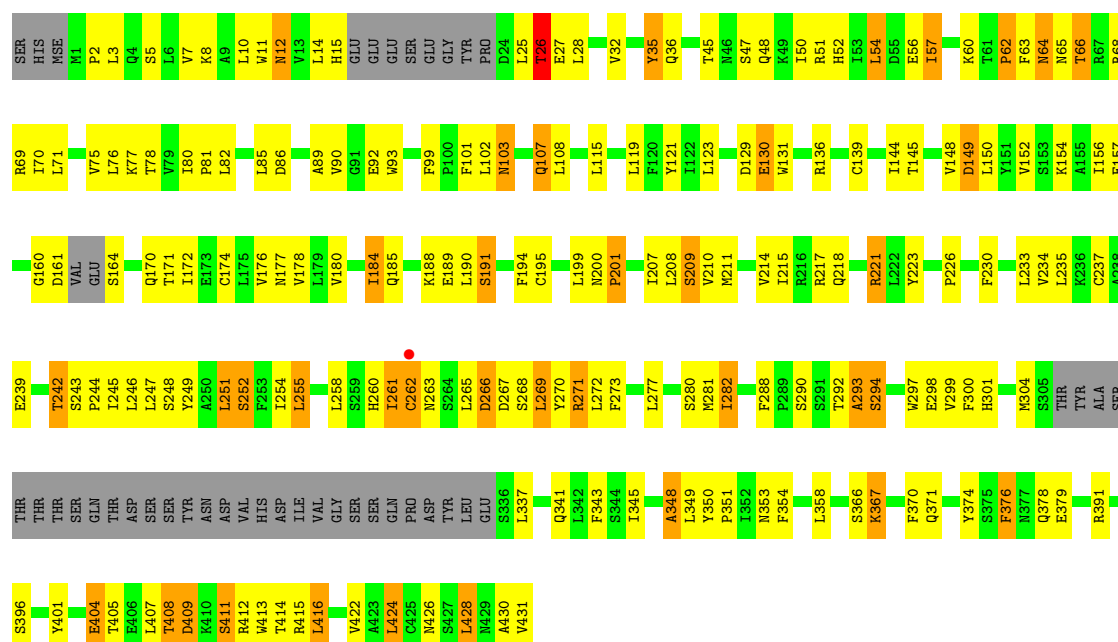
Chain E: 51% 31% 7% 10%





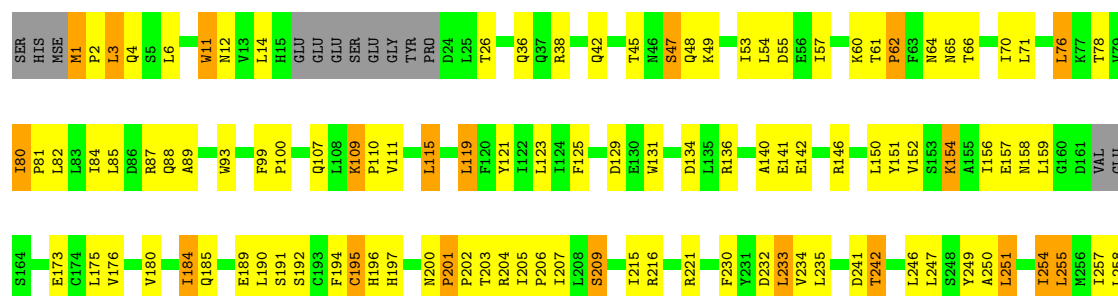
• Molecule 1: Tuberous sclerosis 1 protein homolog

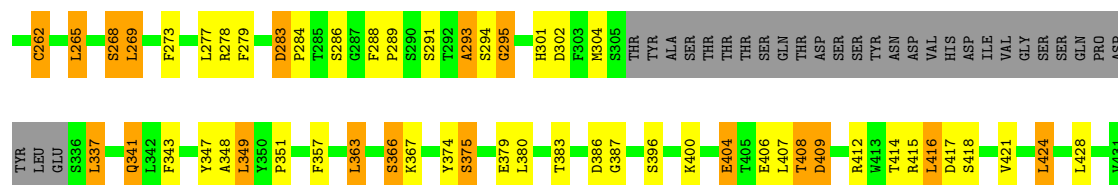
Chain H: 46% 35% 9% 10%



• Molecule 1: Tuberous sclerosis 1 protein homolog

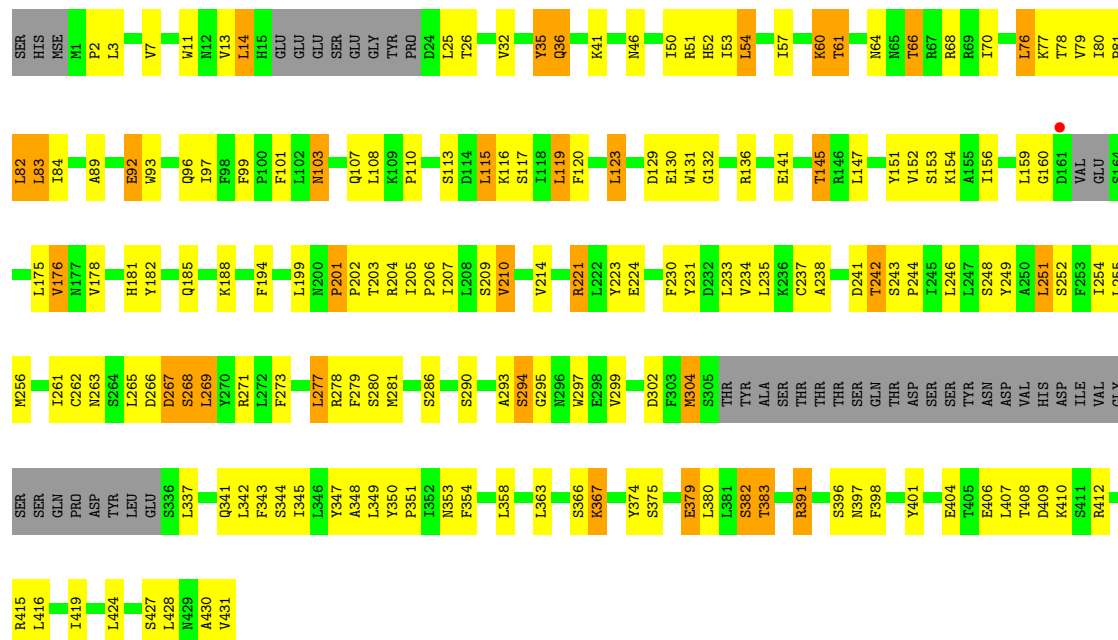
Chain I: 53% 29% 9% 10%





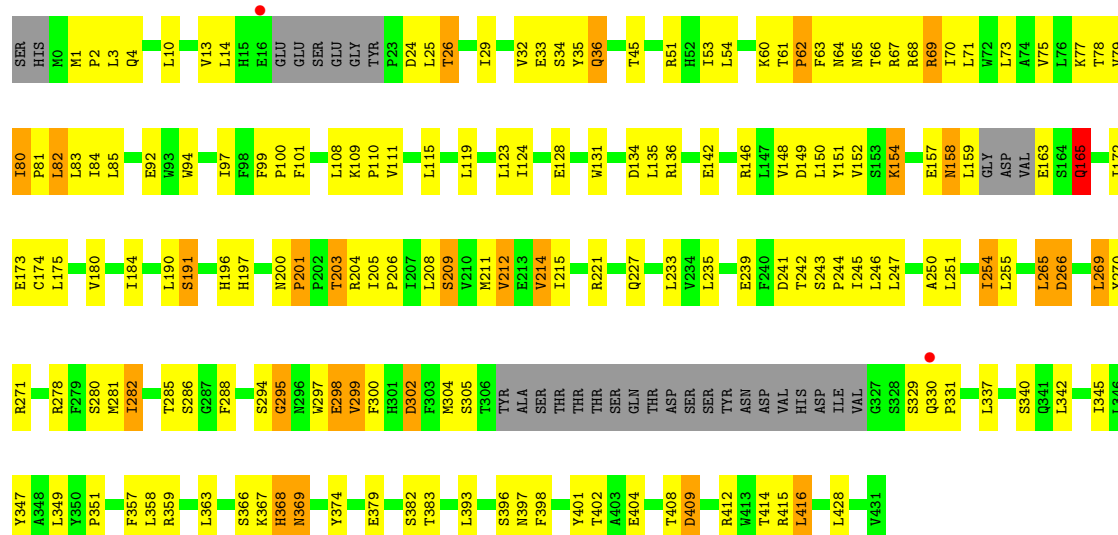
- Molecule 1: Tuberous sclerosis 1 protein homolog

Chain J: 50% 33% 8% 10%

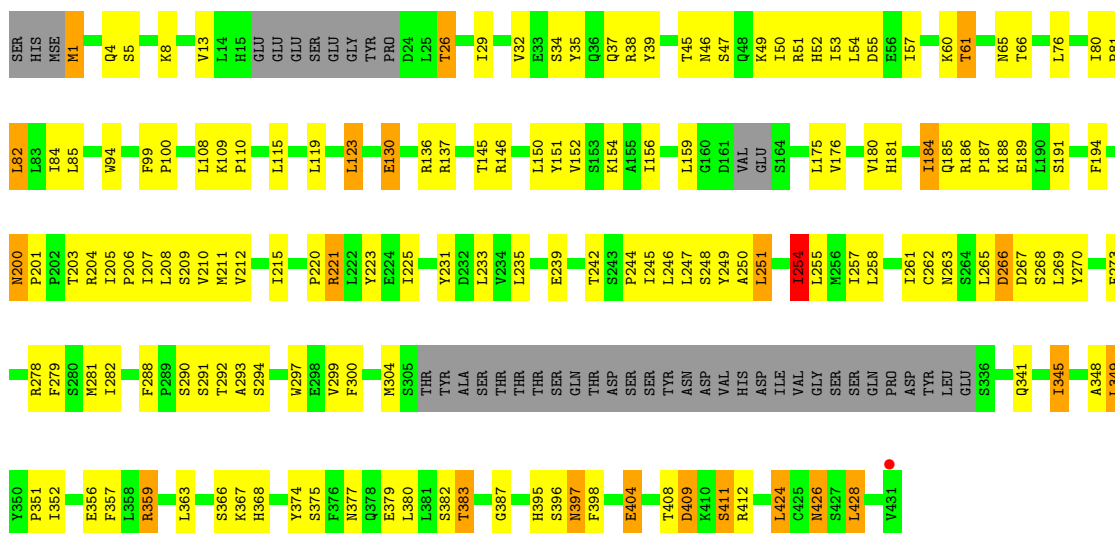


- Molecule 1: Tuberous sclerosis 1 protein homolog

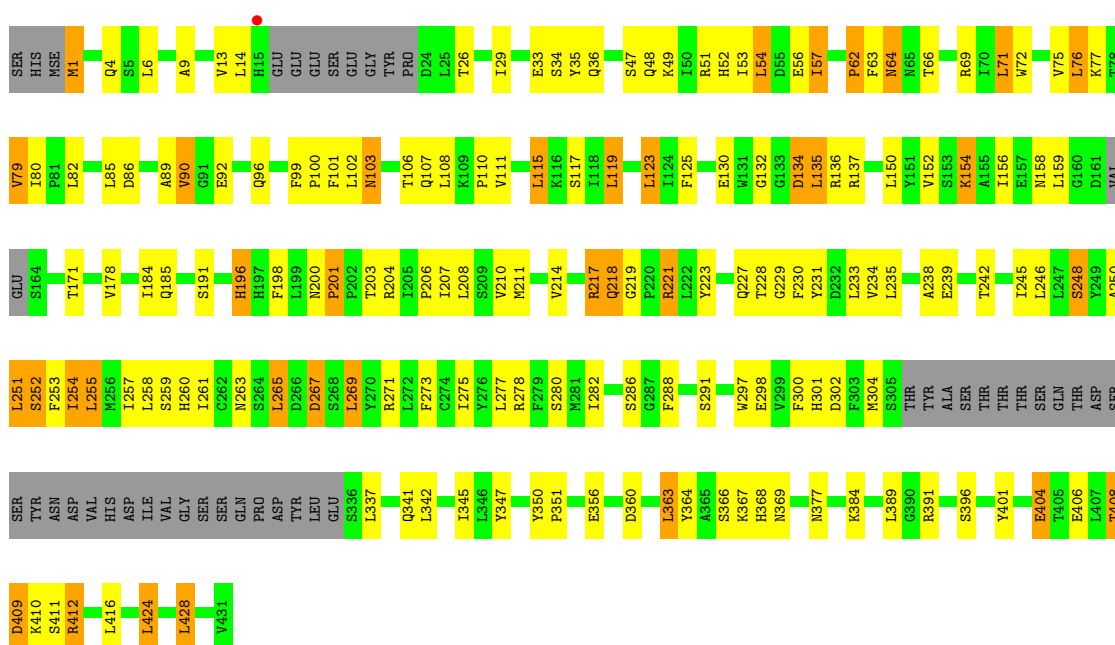
Chain K: 54% 33% 6% 7%



Chain L: 54% 31% 5% 10%

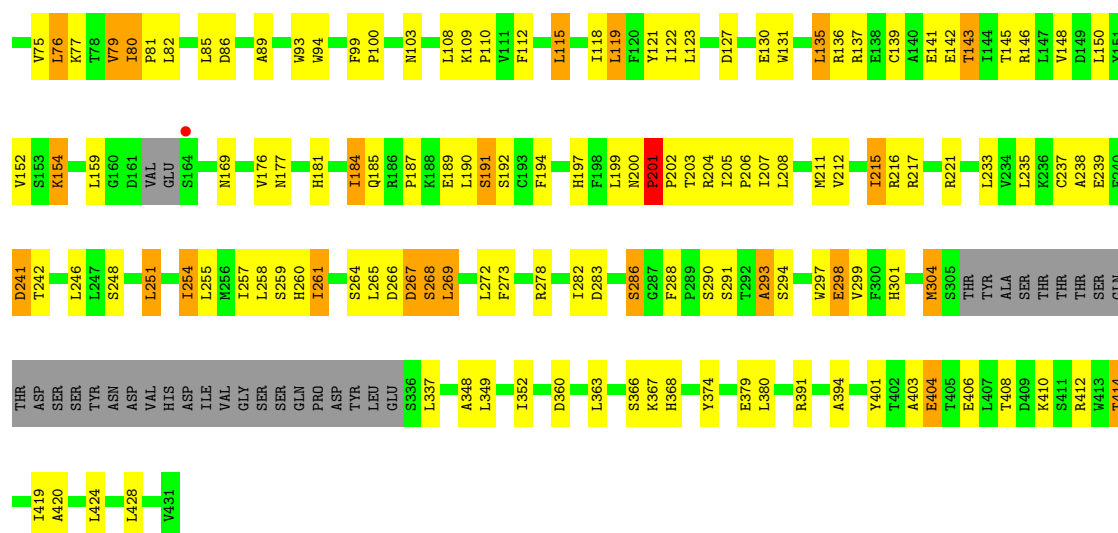


Chain M: 52% 30% 8% 10%

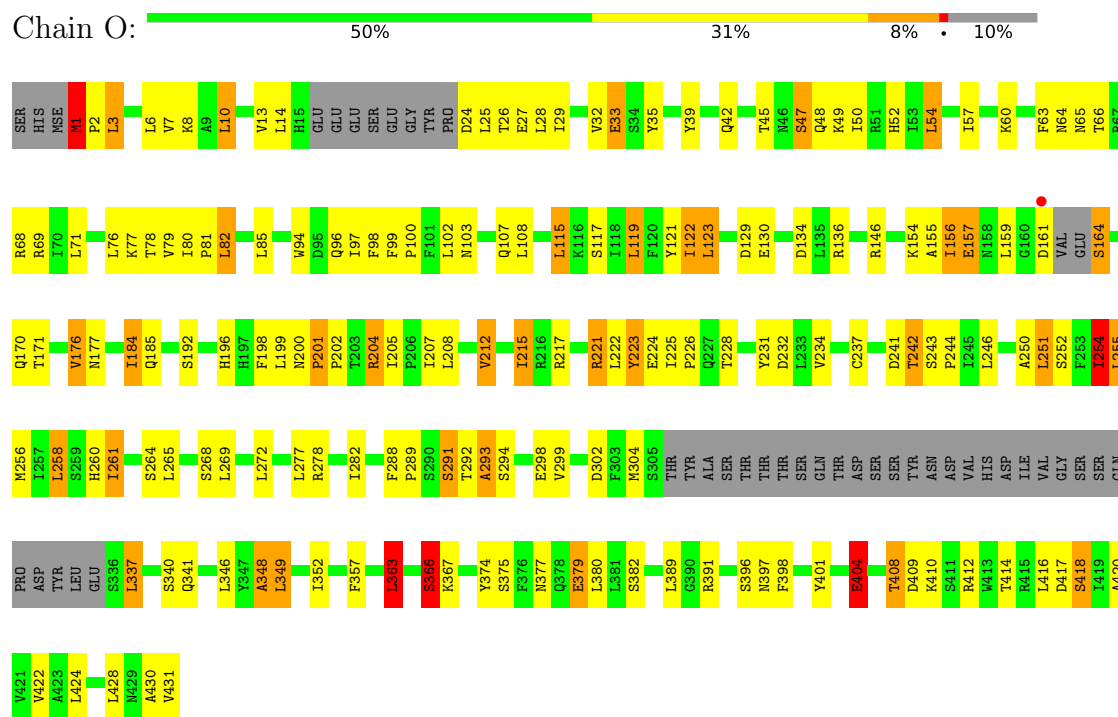


Chain N: 51% 32% 7% 10%

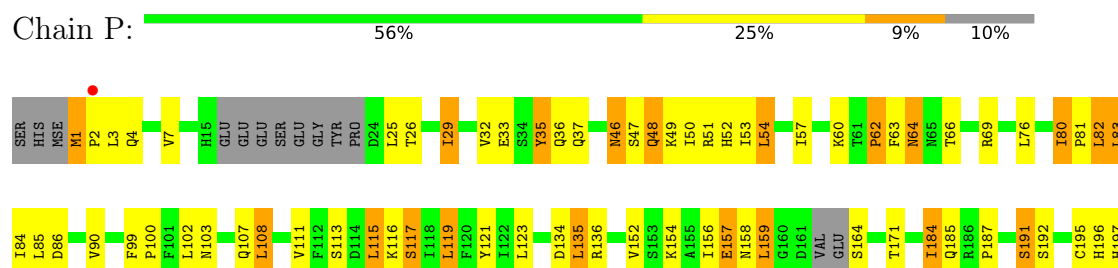


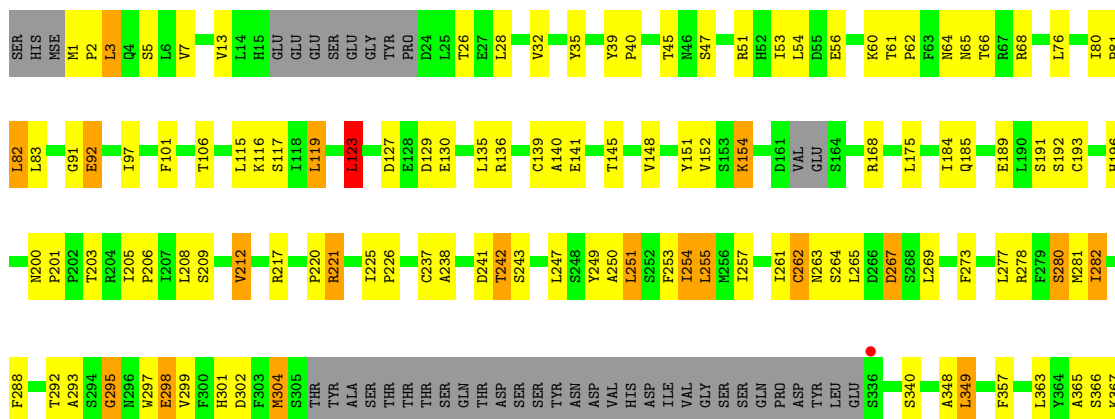


• Molecule 1: Tuberosclerosis 1 protein homolog



• Molecule 1: Tuberosclerosis 1 protein homolog

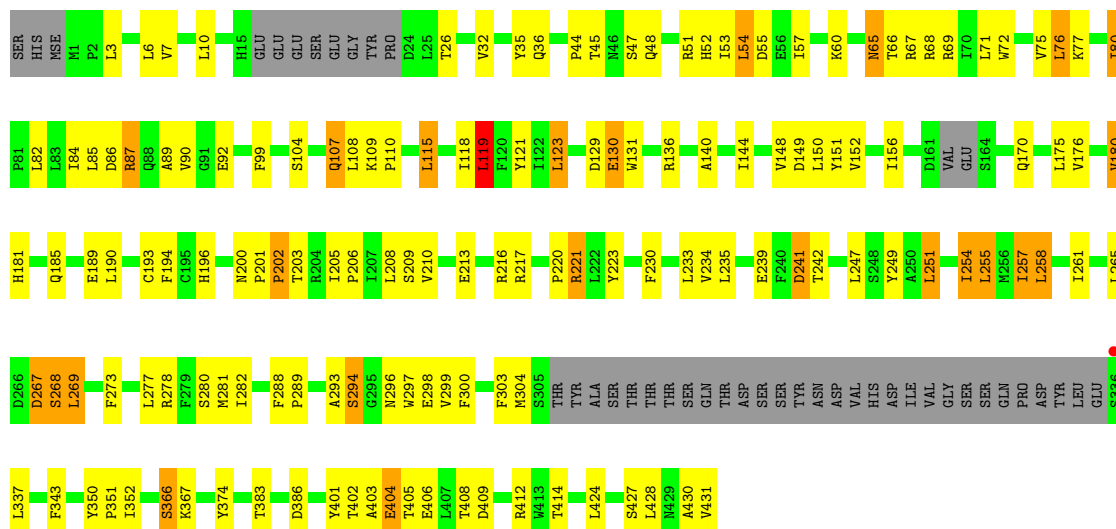






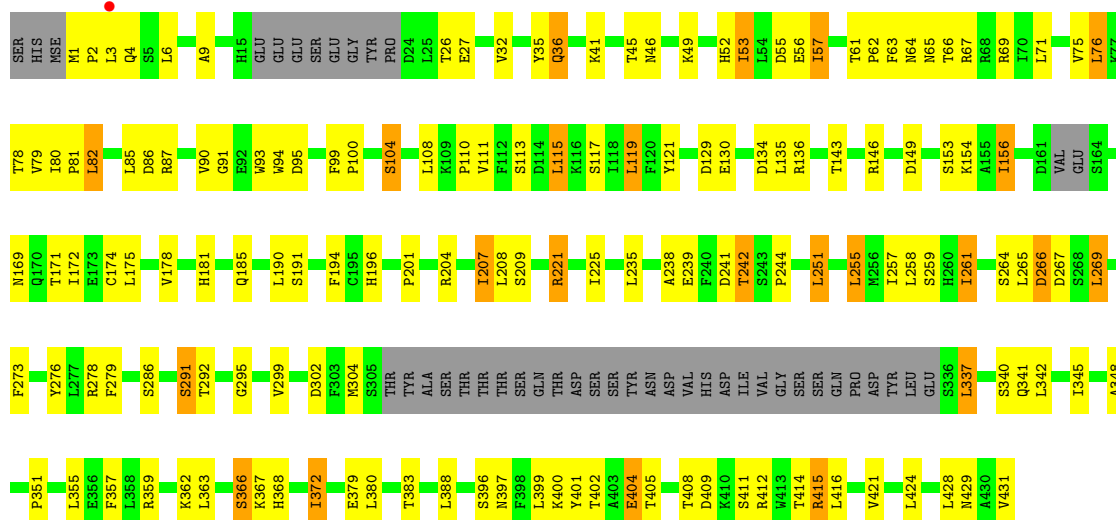
- Molecule 1: Tuberous sclerosis 1 protein homolog

Chain S: 56% 28% 6% 10%



- Molecule 1: Tuberous sclerosis 1 protein homolog

Chain T: 55% 30% 5% 10%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	109.32Å 254.83Å 228.47Å 90.00° 99.71° 90.00°	Depositor
Resolution (Å)	39.82 – 3.30 39.82 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.2 (39.82-3.30) 99.2 (39.82-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.186 , 0.268 0.186 , 0.276	Depositor DCC
R_{free} test set	10003 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	85.9	Xtriage
Anisotropy	0.283	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 53.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	63794	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.87	1/3343 (0.0%)	1.16	15/4535 (0.3%)
1	B	0.88	3/3257 (0.1%)	1.18	14/4421 (0.3%)
1	C	0.88	0/3257	1.14	12/4421 (0.3%)
1	D	0.89	1/3257 (0.0%)	1.15	17/4421 (0.4%)
1	E	0.85	0/3257	1.16	13/4421 (0.3%)
1	F	0.83	0/3257	1.14	14/4421 (0.3%)
1	G	0.88	0/3257	1.16	12/4421 (0.3%)
1	H	0.82	0/3257	1.11	6/4421 (0.1%)
1	I	0.93	0/3257	1.16	10/4421 (0.2%)
1	J	0.86	0/3257	1.16	10/4421 (0.2%)
1	K	0.86	0/3343	1.17	14/4535 (0.3%)
1	L	0.91	1/3257 (0.0%)	1.17	10/4421 (0.2%)
1	M	0.89	0/3257	1.23	20/4421 (0.5%)
1	N	0.92	1/3257 (0.0%)	1.17	9/4421 (0.2%)
1	O	0.96	1/3257 (0.0%)	1.23	17/4421 (0.4%)
1	P	0.87	1/3257 (0.0%)	1.17	13/4421 (0.3%)
1	Q	0.88	0/3257	1.13	10/4421 (0.2%)
1	R	0.86	0/3257	1.14	8/4421 (0.2%)
1	S	0.78	0/3257	1.07	5/4421 (0.1%)
1	T	0.84	0/3257	1.13	11/4421 (0.2%)
All	All	0.88	9/65312 (0.0%)	1.16	240/88648 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1
1	F	0	1
1	I	0	1
1	K	0	1
1	O	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	P	0	1
All	All	0	7

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	201	PRO	CA-C	7.01	1.58	1.52
1	N	80	ILE	CA-C	6.96	1.60	1.52
1	B	205	ILE	CA-CB	6.39	1.57	1.54
1	B	188	LYS	N-CA	5.87	1.53	1.46
1	B	165	GLN	N-CA	5.77	1.53	1.46
1	L	345	ILE	C-O	-5.39	1.17	1.24
1	D	201	PRO	CA-C	5.24	1.57	1.52
1	O	254	ILE	CA-C	5.08	1.59	1.52
1	P	157	GLU	N-CA	5.03	1.52	1.46

All (240) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	304	MSE	CB-CA-C	10.15	128.63	111.68
1	I	201	PRO	N-CA-C	9.95	122.84	110.70
1	A	201	PRO	N-CA-C	9.72	122.55	110.70
1	O	25	LEU	N-CA-C	9.70	124.95	112.34
1	D	201	PRO	N-CA-C	9.53	122.33	110.70
1	M	80	ILE	CA-C-N	-8.91	110.61	119.87
1	M	80	ILE	C-N-CA	-8.91	110.61	119.87
1	R	97	ILE	N-CA-C	8.56	118.38	111.62
1	N	201	PRO	N-CA-C	8.44	120.99	110.70
1	Q	201	PRO	N-CA-C	8.41	120.96	110.70
1	R	201	PRO	N-CA-C	8.39	120.93	110.70
1	C	201	PRO	N-CA-C	8.37	120.91	110.70
1	L	201	PRO	N-CA-C	8.37	120.91	110.70
1	O	201	PRO	N-CA-C	8.28	120.81	110.70
1	E	304	MSE	CB-CA-C	8.27	124.36	111.72
1	O	47	SER	N-CA-C	-8.22	101.91	111.03
1	K	201	PRO	N-CA-C	8.20	120.71	110.70
1	M	156	ILE	N-CA-C	8.05	117.98	111.62
1	P	201	PRO	N-CA-C	7.95	120.40	110.70
1	E	201	PRO	N-CA-C	7.89	120.33	110.70
1	F	201	PRO	CA-C-N	-7.87	111.61	119.56
1	F	201	PRO	C-N-CA	-7.87	111.61	119.56
1	J	201	PRO	N-CA-C	7.85	120.28	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1	MSE	CG-SE-CE	7.76	116.00	98.92
1	H	201	PRO	N-CA-C	7.61	119.98	110.70
1	O	366	SER	N-CA-C	-7.59	100.51	110.53
1	R	123	LEU	N-CA-C	7.43	119.46	111.36
1	E	111	VAL	N-CA-C	-7.40	104.01	110.74
1	M	201	PRO	N-CA-C	7.33	119.64	110.70
1	L	123	LEU	N-CA-C	7.26	118.89	110.97
1	G	201	PRO	N-CA-C	7.24	119.53	110.70
1	F	201	PRO	N-CA-C	7.20	119.49	110.70
1	L	254	ILE	N-CA-C	-7.18	103.53	110.42
1	T	156	ILE	N-CA-C	7.17	118.14	112.12
1	N	360	ASP	CA-C-N	7.14	126.39	118.97
1	N	360	ASP	C-N-CA	7.14	126.39	118.97
1	T	366	SER	N-CA-C	-7.11	100.00	110.52
1	H	200	ASN	CA-C-N	7.07	127.66	120.38
1	H	200	ASN	C-N-CA	7.07	127.66	120.38
1	J	25	LEU	N-CA-C	6.98	121.23	113.21
1	L	225	ILE	CA-C-N	-6.97	112.45	119.56
1	L	225	ILE	C-N-CA	-6.97	112.45	119.56
1	C	113	SER	N-CA-C	-6.94	103.33	111.03
1	T	135	LEU	N-CA-C	6.90	118.80	111.28
1	M	158	ASN	N-CA-C	6.88	121.69	113.16
1	K	97	ILE	CB-CA-C	-6.85	104.95	111.05
1	G	99	PHE	CA-C-N	-6.84	112.58	119.56
1	G	99	PHE	C-N-CA	-6.84	112.58	119.56
1	K	299	VAL	N-CA-C	6.82	118.23	109.30
1	S	273	PHE	N-CA-C	-6.82	103.93	111.36
1	P	375	SER	N-CA-C	-6.80	99.50	110.32
1	M	156	ILE	CB-CA-C	-6.79	105.01	111.05
1	K	330	GLN	CA-C-N	6.70	128.21	119.84
1	K	330	GLN	C-N-CA	6.70	128.21	119.84
1	G	1	MSE	CG-SE-CE	6.68	113.63	98.92
1	B	219	GLY	CA-C-N	-6.63	113.88	120.98
1	B	219	GLY	C-N-CA	-6.63	113.88	120.98
1	B	201	PRO	N-CA-C	6.59	118.73	110.70
1	N	26	THR	N-CA-C	6.57	119.00	111.11
1	B	273	PHE	N-CA-C	-6.54	104.07	111.07
1	R	304	MSE	CB-CA-C	6.49	119.88	111.50
1	O	397	ASN	N-CA-C	-6.48	104.25	111.71
1	F	64	ASN	N-CA-C	6.47	120.92	112.89
1	E	26	THR	N-CA-C	6.46	118.86	111.11
1	D	304	MSE	CB-CA-C	6.41	122.04	112.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	80	ILE	CA-C-N	-6.41	113.12	120.04
1	G	80	ILE	C-N-CA	-6.41	113.12	120.04
1	M	350	TYR	CA-C-N	6.40	126.32	119.28
1	M	350	TYR	C-N-CA	6.40	126.32	119.28
1	D	409	ASP	N-CA-C	-6.37	96.37	107.20
1	M	178	VAL	CB-CA-C	-6.37	103.82	111.97
1	D	80	ILE	CA-C-N	-6.36	113.58	119.82
1	D	80	ILE	C-N-CA	-6.36	113.58	119.82
1	K	214	VAL	N-CA-C	-6.33	105.66	111.67
1	P	156	ILE	N-CA-C	6.32	116.99	111.56
1	M	200	ASN	CA-C-N	6.32	126.89	120.38
1	M	200	ASN	C-N-CA	6.32	126.89	120.38
1	A	200	ASN	CA-C-N	6.31	126.88	120.38
1	A	200	ASN	C-N-CA	6.31	126.88	120.38
1	G	123	LEU	N-CA-C	6.30	118.96	111.71
1	P	283	ASP	CA-C-N	6.30	125.87	119.19
1	P	283	ASP	C-N-CA	6.30	125.87	119.19
1	B	350	TYR	CA-C-N	6.28	126.19	119.28
1	B	350	TYR	C-N-CA	6.28	126.19	119.28
1	I	53	ILE	CB-CA-C	-6.27	103.85	111.88
1	S	366	SER	N-CA-C	-6.25	101.04	110.28
1	P	135	LEU	N-CA-C	6.23	119.73	111.75
1	Q	79	VAL	N-CA-C	6.23	117.17	111.81
1	G	47	SER	N-CA-C	-6.22	103.65	111.11
1	B	156	ILE	CB-CA-C	-6.21	106.43	111.71
1	E	227	GLN	CB-CA-C	-6.19	100.51	110.79
1	G	205	ILE	CA-C-N	-6.19	112.18	119.05
1	G	205	ILE	C-N-CA	-6.19	112.18	119.05
1	A	101	PHE	N-CA-C	6.16	117.67	111.07
1	I	235	LEU	N-CA-C	6.16	118.00	111.28
1	C	348	ALA	N-CA-C	-6.14	102.42	110.53
1	Q	381	LEU	N-CA-C	-6.12	104.52	111.07
1	I	366	SER	N-CA-C	-6.08	101.48	110.48
1	D	200	ASN	CA-C-N	6.06	126.63	120.38
1	D	200	ASN	C-N-CA	6.06	126.63	120.38
1	R	200	ASN	CA-C-N	6.06	126.62	120.38
1	R	200	ASN	C-N-CA	6.06	126.62	120.38
1	P	219	GLY	N-CA-C	-6.04	104.92	112.23
1	D	408	THR	CB-CA-C	-6.03	103.49	111.82
1	Q	200	ASN	CA-C-N	6.03	126.59	120.38
1	Q	200	ASN	C-N-CA	6.03	126.59	120.38
1	J	304	MSE	CB-CA-C	5.97	119.91	111.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	229	GLY	N-CA-C	-5.96	107.60	114.69
1	B	200	ASN	CA-C-N	5.96	126.52	120.38
1	B	200	ASN	C-N-CA	5.96	126.52	120.38
1	I	283	ASP	CA-C-N	5.93	125.81	119.28
1	I	283	ASP	C-N-CA	5.93	125.81	119.28
1	G	271	ARG	N-CA-C	-5.93	104.45	111.03
1	A	330	GLN	CA-C-N	5.92	126.26	119.93
1	A	330	GLN	C-N-CA	5.92	126.26	119.93
1	K	80	ILE	CA-C-N	-5.91	112.82	118.97
1	K	80	ILE	C-N-CA	-5.91	112.82	118.97
1	O	363	LEU	N-CA-C	-5.89	104.50	111.03
1	H	348	ALA	N-CA-C	-5.88	102.72	110.43
1	F	156	ILE	CB-CA-C	-5.87	101.67	111.29
1	M	356	GLU	N-CA-C	-5.85	104.82	111.14
1	M	207	ILE	N-CA-C	5.85	115.97	110.30
1	M	211	MSE	N-CA-CB	5.84	118.48	110.01
1	C	80	ILE	CA-C-N	-5.82	114.12	119.82
1	C	80	ILE	C-N-CA	-5.82	114.12	119.82
1	D	348	ALA	N-CA-C	-5.80	102.87	110.53
1	N	112	PHE	N-CA-C	-5.80	104.92	112.23
1	A	366	SER	N-CA-C	-5.78	102.49	110.35
1	J	350	TYR	CA-C-N	5.76	124.96	118.97
1	J	350	TYR	C-N-CA	5.76	124.96	118.97
1	D	195	CYS	N-CA-C	5.73	119.37	112.38
1	T	111	VAL	N-CA-C	-5.72	105.15	110.53
1	R	135	LEU	N-CA-C	5.71	118.24	111.33
1	A	80	ILE	CA-C-N	-5.70	113.31	119.24
1	A	80	ILE	C-N-CA	-5.70	113.31	119.24
1	E	156	ILE	CB-CA-C	-5.69	105.33	110.91
1	F	200	ASN	CA-C-N	5.69	126.24	120.38
1	F	200	ASN	C-N-CA	5.69	126.24	120.38
1	S	80	ILE	CA-C-N	-5.69	113.95	119.87
1	S	80	ILE	C-N-CA	-5.69	113.95	119.87
1	Q	366	SER	N-CA-C	-5.68	103.42	110.41
1	L	215	ILE	CB-CA-C	-5.66	104.50	112.14
1	O	348	ALA	N-CA-C	-5.66	102.88	110.24
1	E	203	THR	N-CA-C	5.66	119.44	112.54
1	T	348	ALA	N-CA-C	-5.66	102.66	110.35
1	H	376	PHE	N-CA-C	5.64	117.11	108.42
1	M	245	ILE	N-CA-C	-5.62	105.14	110.42
1	G	53	ILE	CB-CA-C	-5.61	104.70	111.88
1	M	196	HIS	N-CA-CB	5.61	118.14	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	258	LEU	N-CA-C	5.60	117.47	111.36
1	J	210	VAL	CB-CA-C	-5.59	104.51	112.22
1	Q	188	LYS	N-CA-C	-5.57	104.42	111.11
1	P	195	CYS	N-CA-C	5.57	117.43	111.36
1	T	207	ILE	CB-CA-C	-5.56	104.85	111.97
1	O	404	GLU	N-CA-CB	5.53	118.44	110.20
1	I	11	TRP	N-CA-C	-5.53	104.89	111.03
1	E	221	ARG	N-CA-C	-5.53	95.52	111.00
1	F	271	ARG	N-CA-C	-5.53	105.33	111.36
1	E	258	LEU	N-CA-C	5.51	118.21	111.82
1	C	6	LEU	N-CA-C	-5.50	105.36	111.36
1	C	186	ARG	CA-C-N	-5.50	112.94	119.05
1	C	186	ARG	C-N-CA	-5.50	112.94	119.05
1	Q	276	TYR	N-CA-C	-5.49	105.19	111.07
1	M	79	VAL	CB-CA-C	-5.49	106.03	111.30
1	K	165	GLN	N-CA-C	5.48	122.46	110.80
1	A	180	VAL	CB-CA-C	-5.47	104.76	112.14
1	K	53	ILE	CB-CA-C	-5.47	104.70	111.70
1	O	159	LEU	N-CA-C	5.46	122.42	110.80
1	T	156	ILE	CB-CA-C	-5.45	105.57	110.91
1	A	348	ALA	N-CA-C	-5.44	103.45	110.19
1	J	391	ARG	N-CA-C	-5.42	106.35	113.17
1	P	25	LEU	N-CA-C	5.41	119.94	113.23
1	B	358	LEU	N-CA-C	-5.37	102.93	110.50
1	C	165	GLN	N-CA-C	-5.36	106.42	113.12
1	J	160	GLY	N-CA-C	5.36	119.34	110.97
1	M	103	ASN	N-CA-C	5.35	116.80	111.07
1	O	122	ILE	CB-CA-C	-5.35	105.07	112.24
1	A	64	ASN	N-CA-C	5.35	122.19	110.80
1	D	227	GLN	N-CA-C	5.34	118.59	111.75
1	A	375	SER	N-CA-C	-5.33	101.77	110.20
1	R	92	GLU	CA-CB-CG	5.33	124.75	114.10
1	F	122	ILE	CB-CA-C	-5.28	105.12	112.04
1	S	217	ARG	N-CA-C	5.27	119.19	112.34
1	O	1	MSE	CG-SE-CE	5.27	110.51	98.92
1	T	201	PRO	N-CA-C	5.27	117.12	110.70
1	L	387	GLY	N-CA-C	-5.26	106.39	112.50
1	D	44	PRO	N-CA-C	5.25	120.74	113.65
1	J	188	LYS	N-CA-C	-5.25	105.56	111.28
1	P	227	GLN	CB-CA-C	-5.25	100.28	110.46
1	F	92	GLU	CA-CB-CG	5.25	124.59	114.10
1	B	116	LYS	N-CA-C	-5.24	105.26	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	227	GLN	CB-CA-C	-5.22	100.97	110.63
1	P	80	ILE	CA-C-N	-5.22	113.54	119.28
1	P	80	ILE	C-N-CA	-5.22	113.54	119.28
1	H	271	ARG	N-CA-C	-5.21	105.29	110.97
1	F	349	LEU	N-CA-C	5.21	121.89	110.80
1	O	123	LEU	N-CA-C	5.21	117.75	111.40
1	L	352	ILE	N-CA-C	5.21	115.42	110.53
1	J	277	LEU	N-CA-C	-5.20	104.68	111.02
1	B	408	THR	N-CA-C	5.18	117.88	107.41
1	C	260	HIS	CB-CA-C	-5.17	104.86	111.22
1	B	225	ILE	CB-CA-C	-5.17	108.87	114.35
1	N	169	ASN	N-CA-C	5.17	116.61	111.07
1	T	225	ILE	CB-CA-C	-5.17	108.87	114.35
1	K	69	ARG	N-CA-C	-5.16	105.55	111.07
1	P	347	TYR	N-CA-C	-5.16	105.74	111.36
1	E	121	TYR	N-CA-C	-5.16	105.84	111.82
1	I	380	LEU	N-CA-C	5.15	116.90	111.28
1	A	123	LEU	N-CA-C	5.15	117.63	111.71
1	F	406	GLU	N-CA-C	-5.15	105.36	110.97
1	E	288	PHE	CA-C-N	-5.15	114.46	119.76
1	E	288	PHE	C-N-CA	-5.15	114.46	119.76
1	E	401	TYR	N-CA-C	5.14	117.49	109.52
1	L	200	ASN	CA-C-N	5.14	125.67	120.38
1	L	200	ASN	C-N-CA	5.14	125.67	120.38
1	D	43	ASN	CA-C-N	5.13	124.93	119.28
1	D	43	ASN	C-N-CA	5.13	124.93	119.28
1	K	203	THR	CB-CA-C	-5.13	100.51	110.46
1	Q	203	THR	CB-CA-C	-5.13	100.82	110.67
1	O	346	LEU	N-CA-C	5.12	117.77	111.82
1	O	204	ARG	N-CA-C	5.12	117.52	111.33
1	K	416	LEU	N-CA-C	5.11	117.24	111.11
1	C	184	ILE	N-CA-C	-5.10	104.90	112.04
1	I	80	ILE	N-CA-CB	5.09	113.71	110.50
1	T	204	ARG	N-CA-C	5.08	116.51	110.97
1	D	221	ARG	N-CA-C	-5.08	96.78	111.00
1	F	14	LEU	N-CA-C	5.08	118.31	112.57
1	D	125	PHE	N-CA-C	5.06	117.08	109.23
1	D	366	SER	N-CA-C	-5.06	103.85	110.53
1	B	9	ALA	N-CA-C	5.06	117.53	111.71
1	K	135	LEU	N-CA-C	5.05	117.17	111.11
1	T	53	ILE	CB-CA-C	-5.05	105.51	111.97
1	A	212	VAL	N-CA-CB	5.04	117.39	110.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	200	ASN	CA-C-N	5.03	125.56	120.38
1	N	200	ASN	C-N-CA	5.03	125.56	120.38
1	F	242	THR	N-CA-CB	-5.02	104.23	110.90
1	O	302	ASP	CA-C-N	-5.01	116.10	122.77
1	O	302	ASP	C-N-CA	-5.01	116.10	122.77
1	I	38	ARG	N-CA-C	-5.01	107.33	113.50
1	Q	156	ILE	N-CA-C	5.01	115.96	111.90

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	220	PRO	Peptide
1	F	164	SER	Peptide
1	I	3	LEU	Peptide
1	K	368	HIS	Peptide
1	O	164	SER	Peptide
1	O	24	ASP	Peptide
1	P	164	SER	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3268	0	3216	111	0
1	B	3181	0	3145	92	0
1	C	3181	0	3145	78	0
1	D	3181	0	3145	83	0
1	E	3181	0	3145	86	0
1	F	3181	0	3145	87	0
1	G	3181	0	3145	83	0
1	H	3181	0	3145	126	0
1	I	3181	0	3145	84	0
1	J	3181	0	3145	101	0
1	K	3268	0	3216	91	0
1	L	3181	0	3145	89	0
1	M	3181	0	3145	103	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N	3181	0	3145	102	0
1	O	3181	0	3145	95	0
1	P	3181	0	3145	83	0
1	Q	3181	0	3145	91	0
1	R	3181	0	3145	79	0
1	S	3181	0	3145	92	0
1	T	3181	0	3145	79	0
All	All	63794	0	63042	1750	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (1750) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:115:LEU:HD22	1:G:119:LEU:HD22	1.43	0.98
1:M:401:TYR:CZ	1:M:412:ARG:HG3	1.99	0.96
1:A:121:TYR:O	1:A:136:ARG:NH2	2.05	0.90
1:I:142:GLU:OE2	1:I:146:ARG:NH1	2.08	0.86
1:Q:279:PHE:O	1:Q:282:ILE:HG22	1.76	0.85
1:E:235:LEU:O	1:E:239:GLU:HG3	1.77	0.85
1:F:250:ALA:O	1:F:254:ILE:HG23	1.77	0.85
1:T:185:GLN:O	1:T:221:ARG:NH2	2.09	0.85
1:J:32:VAL:HG13	1:J:82:LEU:HD21	1.59	0.85
1:L:130:GLU:OE1	1:L:136:ARG:NH1	2.11	0.83
1:R:401:TYR:CZ	1:R:412:ARG:HG3	2.13	0.83
1:R:379:GLU:HG3	1:T:185:GLN:HA	1.58	0.82
1:M:185:GLN:HA	1:O:379:GLU:HG3	1.60	0.82
1:G:299:VAL:HG11	1:G:301:HIS:CE1	2.15	0.81
1:J:89:ALA:O	1:J:92:GLU:HB2	1.81	0.81
1:P:379:GLU:HG3	1:R:185:GLN:HA	1.60	0.81
1:L:379:GLU:HG3	1:N:185:GLN:HA	1.63	0.80
1:B:406:GLU:O	1:B:412:ARG:NH2	2.13	0.80
1:H:251:LEU:HD22	1:H:255:LEU:HD22	1.64	0.80
1:R:299:VAL:HG11	1:R:301:HIS:CE1	2.18	0.79
1:N:199:LEU:O	1:N:201:PRO:HD3	1.84	0.78
1:S:401:TYR:CZ	1:S:412:ARG:HG3	2.19	0.78
1:S:44:PRO:O	1:S:48:GLN:HG2	1.84	0.77
1:B:366:SER:O	1:B:367:LYS:HB2	1.83	0.77
1:L:409:ASP:OD1	1:L:411:SER:OG	2.01	0.77
1:L:282:ILE:HD12	1:L:288:PHE:CZ	2.20	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:402:THR:OG1	1:T:405:THR:HG23	1.84	0.77
1:C:235:LEU:O	1:C:239:GLU:HG3	1.85	0.76
1:M:115:LEU:HD22	1:M:119:LEU:HD22	1.68	0.76
1:N:115:LEU:HD22	1:N:119:LEU:HD22	1.66	0.76
1:P:50:ILE:O	1:P:54:LEU:HD22	1.86	0.76
1:H:366:SER:O	1:H:367:LYS:HB2	1.85	0.76
1:M:71:LEU:O	1:M:75:VAL:HG23	1.85	0.76
1:G:185:GLN:HA	1:I:379:GLU:HG3	1.68	0.76
1:I:14:LEU:HD23	1:I:71:LEU:HD23	1.67	0.75
1:S:32:VAL:O	1:S:36:GLN:HG3	1.86	0.75
1:J:278:ARG:HD2	1:J:374:TYR:CZ	2.20	0.75
1:H:89:ALA:O	1:H:92:GLU:N	2.19	0.75
1:O:222:LEU:O	1:O:224:GLU:N	2.20	0.75
1:O:401:TYR:CZ	1:O:412:ARG:HG3	2.21	0.75
1:J:115:LEU:HD22	1:J:119:LEU:HD22	1.68	0.75
1:K:180:VAL:HG13	1:K:214:VAL:HG22	1.67	0.74
1:Q:278:ARG:HD2	1:Q:374:TYR:CE1	2.22	0.74
1:A:379:GLU:HG3	1:I:185:GLN:HA	1.68	0.74
1:Q:152:VAL:HG13	1:Q:203:THR:HG22	1.69	0.74
1:H:99:PHE:O	1:H:103:ASN:HB2	1.88	0.74
1:J:130:GLU:OE1	1:J:136:ARG:NH1	2.21	0.74
1:J:280:SER:O	1:J:281:MSE:HE2	1.87	0.73
1:L:366:SER:O	1:L:367:LYS:HB2	1.89	0.73
1:L:185:GLN:HA	1:T:379:GLU:HG3	1.70	0.73
1:O:102:LEU:O	1:O:171:THR:HG23	1.88	0.73
1:N:121:TYR:O	1:N:136:ARG:NH2	2.21	0.73
1:G:3:LEU:O	1:G:7:VAL:HG23	1.89	0.73
1:L:404:GLU:O	1:L:408:THR:HG22	1.88	0.73
1:O:185:GLN:HA	1:Q:379:GLU:HG3	1.69	0.73
1:P:47:SER:O	1:P:51:ARG:HG3	1.89	0.73
1:G:401:TYR:CZ	1:G:412:ARG:HG3	2.24	0.72
1:J:152:VAL:HG13	1:J:203:THR:HG22	1.69	0.72
1:K:250:ALA:O	1:K:254:ILE:HG23	1.89	0.72
1:T:404:GLU:O	1:T:408:THR:HG22	1.88	0.72
1:N:261:ILE:HG21	1:N:264:SER:HB2	1.70	0.72
1:O:161:ASP:CB	1:O:164:SER:CB	2.67	0.72
1:F:243:SER:OG	1:F:302:ASP:OD1	2.07	0.72
1:M:255:LEU:HD23	1:M:337:LEU:HB3	1.70	0.72
1:N:51:ARG:HA	1:N:54:LEU:HD23	1.70	0.71
1:G:150:LEU:O	1:G:154:LYS:HB2	1.90	0.71
1:T:255:LEU:HD23	1:T:337:LEU:HD12	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:235:LEU:O	1:M:239:GLU:HG3	1.91	0.71
1:L:278:ARG:HD2	1:L:374:TYR:CZ	2.26	0.71
1:R:293:ALA:HB3	1:R:373:ARG:NE	2.06	0.71
1:S:151:TYR:HA	1:S:175:LEU:HD13	1.72	0.70
1:H:211:MSE:O	1:H:215:ILE:HG12	1.92	0.70
1:N:10:LEU:O	1:N:13:VAL:HG12	1.92	0.70
1:G:414:THR:HG21	1:H:223:TYR:CE2	2.27	0.69
1:G:71:LEU:O	1:G:75:VAL:HG23	1.91	0.69
1:K:158:ASN:OD1	1:K:158:ASN:N	2.25	0.69
1:A:278:ARG:HD2	1:A:374:TYR:CE1	2.27	0.69
1:C:250:ALA:O	1:C:254:ILE:HG23	1.92	0.69
1:N:235:LEU:O	1:N:239:GLU:HG3	1.92	0.69
1:I:1:MSE:HE2	1:I:4:GLN:HB2	1.74	0.69
1:A:238:ALA:O	1:A:278:ARG:NH1	2.26	0.69
1:P:430:ALA:O	1:P:431:VAL:HB	1.92	0.69
1:Q:32:VAL:HG13	1:Q:82:LEU:HD21	1.75	0.68
1:M:251:LEU:HD22	1:M:255:LEU:HD22	1.75	0.68
1:J:401:TYR:CZ	1:J:412:ARG:HG3	2.28	0.68
1:P:401:TYR:OH	1:P:412:ARG:HG3	1.94	0.68
1:B:358:LEU:O	1:B:359:ARG:CB	2.42	0.68
1:G:406:GLU:O	1:G:412:ARG:NH2	2.27	0.68
1:R:243:SER:OG	1:R:302:ASP:OD1	2.09	0.68
1:P:247:LEU:HD12	1:P:288:PHE:CD1	2.29	0.67
1:A:29:ILE:O	1:A:33:GLU:HG3	1.95	0.67
1:C:404:GLU:O	1:C:408:THR:HG22	1.95	0.67
1:R:293:ALA:HB3	1:R:373:ARG:HE	1.60	0.67
1:L:247:LEU:HD12	1:L:288:PHE:CD1	2.29	0.67
1:H:194:PHE:CD1	1:H:207:ILE:HG23	2.29	0.67
1:R:250:ALA:O	1:R:254:ILE:HG23	1.95	0.67
1:C:235:LEU:O	1:C:239:GLU:CG	2.43	0.67
1:G:32:VAL:HG13	1:G:82:LEU:HD21	1.76	0.67
1:K:163:GLU:C	1:K:165:GLN:N	2.52	0.66
1:D:102:LEU:O	1:D:105:PRO:HD3	1.95	0.66
1:E:401:TYR:CZ	1:E:412:ARG:HG3	2.31	0.66
1:S:408:THR:HG23	1:S:408:THR:O	1.96	0.66
1:B:401:TYR:CZ	1:B:412:ARG:HG3	2.31	0.66
1:D:277:LEU:HD23	1:D:277:LEU:C	2.21	0.66
1:H:255:LEU:HD23	1:H:337:LEU:HB3	1.77	0.66
1:K:66:THR:O	1:K:67:ARG:C	2.39	0.66
1:J:96:GLN:O	1:J:97:ILE:HD13	1.97	0.65
1:I:241:ASP:O	1:I:278:ARG:NH2	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:241:ASP:HA	1:T:299:VAL:HG13	1.77	0.65
1:B:348:ALA:O	1:B:350:TYR:N	2.29	0.65
1:L:1:MSE:HE2	1:L:4:GLN:HB2	1.78	0.65
1:F:401:TYR:CZ	1:F:412:ARG:HG3	2.32	0.65
1:H:401:TYR:CZ	1:H:412:ARG:HG3	2.32	0.65
1:B:115:LEU:HD22	1:B:119:LEU:HD22	1.77	0.65
1:O:156:ILE:HG22	1:O:157:GLU:H	1.62	0.65
1:C:47:SER:O	1:C:51:ARG:HG3	1.97	0.65
1:C:278:ARG:HD2	1:C:374:TYR:CZ	2.32	0.65
1:O:250:ALA:O	1:O:254:ILE:HG23	1.95	0.65
1:S:89:ALA:O	1:S:92:GLU:HB2	1.96	0.65
1:H:180:VAL:O	1:H:184:ILE:HG23	1.95	0.65
1:J:382:SER:O	1:J:383:THR:C	2.40	0.65
1:L:379:GLU:CG	1:N:185:GLN:HA	2.26	0.65
1:R:238:ALA:O	1:R:278:ARG:NH1	2.30	0.65
1:E:27:GLU:O	1:E:30:ALA:HB3	1.97	0.64
1:B:69:ARG:O	1:B:70:ILE:C	2.40	0.64
1:E:84:ILE:C	1:E:85:LEU:HD12	2.23	0.64
1:O:80:ILE:N	1:O:81:PRO:HD2	2.12	0.64
1:E:71:LEU:O	1:E:75:VAL:HG23	1.98	0.64
1:E:225:ILE:O	1:E:228:THR:OG1	2.16	0.64
1:H:366:SER:O	1:H:367:LYS:CB	2.45	0.64
1:G:191:SER:HB2	1:G:228:THR:HG21	1.78	0.64
1:K:24:ASP:OD1	1:K:26:THR:OG1	2.13	0.64
1:N:264:SER:O	1:N:268:SER:OG	2.16	0.64
1:C:366:SER:O	1:C:367:LYS:HB2	1.98	0.64
1:I:109:LYS:HB2	1:I:110:PRO:HD3	1.77	0.64
1:K:278:ARG:HD2	1:K:374:TYR:CE1	2.33	0.64
1:O:3:LEU:O	1:O:7:VAL:HG23	1.99	0.63
1:I:150:LEU:HG	1:I:175:LEU:HD11	1.81	0.63
1:M:134:ASP:O	1:M:136:ARG:N	2.31	0.63
1:K:99:PHE:HB3	1:K:100:PRO:HD3	1.80	0.63
1:B:115:LEU:HD22	1:B:119:LEU:CD2	2.28	0.63
1:T:273:PHE:HB3	1:T:357:PHE:CE2	2.33	0.63
1:H:102:LEU:O	1:H:171:THR:HG23	1.99	0.63
1:K:347:TYR:O	1:K:351:PRO:HB3	1.99	0.63
1:L:291:SER:OG	1:L:292:THR:N	2.31	0.63
1:L:366:SER:O	1:L:367:LYS:CB	2.45	0.63
1:I:76:LEU:HG	1:I:93:TRP:CZ3	2.34	0.63
1:J:406:GLU:O	1:J:412:ARG:NH2	2.31	0.63
1:B:379:GLU:HG3	1:D:185:GLN:HA	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:115:LEU:HD22	1:E:119:LEU:HD22	1.80	0.63
1:M:53:ILE:O	1:M:57:ILE:HG13	1.99	0.63
1:M:401:TYR:OH	1:M:412:ARG:CG	2.47	0.63
1:C:144:ILE:O	1:C:148:VAL:HG23	1.98	0.63
1:E:200:ASN:OD1	1:E:202:PRO:HD2	1.99	0.63
1:L:32:VAL:HG13	1:L:82:LEU:HD21	1.80	0.62
1:Q:278:ARG:HD2	1:Q:374:TYR:CZ	2.34	0.62
1:L:200:ASN:O	1:L:203:THR:OG1	2.15	0.62
1:P:1:MSE:HE2	1:P:4:GLN:HB2	1.81	0.62
1:K:379:GLU:HG3	1:S:185:GLN:HA	1.81	0.62
1:O:156:ILE:HG22	1:O:157:GLU:N	2.13	0.62
1:F:404:GLU:O	1:F:408:THR:HG22	1.99	0.62
1:J:366:SER:O	1:J:367:LYS:HB2	2.00	0.62
1:N:70:ILE:HD11	1:N:108:LEU:HD12	1.82	0.62
1:N:142:GLU:OE2	1:N:146:ARG:NH1	2.32	0.62
1:R:152:VAL:HG13	1:R:203:THR:HG22	1.79	0.62
1:S:404:GLU:O	1:S:408:THR:HG22	2.00	0.62
1:R:148:VAL:HG21	1:R:193:CYS:HB3	1.82	0.62
1:B:366:SER:O	1:B:367:LYS:CB	2.47	0.62
1:K:280:SER:O	1:K:281:MSE:HE2	1.99	0.62
1:T:414:THR:C	1:T:416:LEU:H	2.08	0.62
1:P:215:ILE:HD12	1:P:222:LEU:HD22	1.82	0.62
1:A:144:ILE:O	1:A:148:VAL:HG23	2.00	0.62
1:F:262:CYS:HA	1:F:265:LEU:HD12	1.81	0.62
1:M:198:PHE:CE1	1:M:204:ARG:HG2	2.35	0.61
1:J:293:ALA:O	1:J:294:SER:HB3	1.98	0.61
1:F:239:GLU:O	1:F:278:ARG:NH1	2.34	0.61
1:N:86:ASP:H	1:N:89:ALA:HB3	1.65	0.61
1:E:243:SER:OG	1:E:302:ASP:OD1	2.15	0.61
1:H:64:ASN:OD1	1:H:64:ASN:N	2.30	0.61
1:I:152:VAL:HG13	1:I:203:THR:HG22	1.80	0.61
1:T:340:SER:HB2	1:T:388:LEU:HD21	1.83	0.61
1:B:148:VAL:HG21	1:B:193:CYS:HB3	1.81	0.61
1:E:366:SER:O	1:E:367:LYS:HB2	2.01	0.61
1:E:410:LYS:N	1:E:410:LYS:HD3	2.15	0.61
1:L:396:SER:O	1:L:398:PHE:N	2.33	0.61
1:I:406:GLU:O	1:I:412:ARG:NH2	2.34	0.61
1:K:63:PHE:CE1	1:K:69:ARG:HA	2.36	0.61
1:N:28:LEU:O	1:N:32:VAL:HG23	2.01	0.61
1:A:366:SER:O	1:A:367:LYS:HB2	2.01	0.61
1:O:184:ILE:HD11	1:Q:380:LEU:HB2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:130:GLU:OE1	1:R:136:ARG:NH1	2.33	0.61
1:R:366:SER:O	1:R:367:LYS:HB2	2.01	0.61
1:F:278:ARG:HD2	1:F:374:TYR:CE1	2.36	0.61
1:M:401:TYR:OH	1:M:412:ARG:HG3	2.00	0.61
1:S:430:ALA:O	1:S:431:VAL:HB	2.01	0.61
1:A:194:PHE:CD1	1:A:207:ILE:HG23	2.36	0.61
1:A:262:CYS:SG	1:B:421:VAL:HG21	2.41	0.61
1:R:141:GLU:O	1:R:145:THR:OG1	2.17	0.61
1:K:25:LEU:O	1:K:26:THR:C	2.43	0.60
1:O:255:LEU:HD23	1:O:337:LEU:HB3	1.82	0.60
1:N:150:LEU:O	1:N:154:LYS:HB2	2.01	0.60
1:T:235:LEU:O	1:T:239:GLU:HG3	2.00	0.60
1:A:401:TYR:CZ	1:A:412:ARG:HG3	2.36	0.60
1:D:283:ASP:OD1	1:D:284:PRO:CD	2.49	0.60
1:D:360:ASP:OD2	1:D:363:LEU:HB2	2.01	0.60
1:H:130:GLU:OE1	1:H:136:ARG:NH1	2.34	0.60
1:H:239:GLU:OE2	1:H:271:ARG:NE	2.31	0.60
1:I:250:ALA:O	1:I:254:ILE:HG23	2.02	0.60
1:B:76:LEU:HG	1:B:93:TRP:CZ3	2.36	0.60
1:I:151:TYR:HA	1:I:175:LEU:HD13	1.84	0.60
1:J:205:ILE:HB	1:J:206:PRO:HD3	1.84	0.60
1:L:49:LYS:O	1:L:53:ILE:HG12	2.01	0.60
1:O:32:VAL:HG13	1:O:82:LEU:HD21	1.84	0.60
1:A:7:VAL:HG13	1:A:53:ILE:HG21	1.83	0.60
1:C:184:ILE:HD11	1:E:380:LEU:HB2	1.83	0.60
1:J:64:ASN:OD1	1:J:68:ARG:NH1	2.35	0.60
1:L:282:ILE:HD12	1:L:288:PHE:CE2	2.36	0.60
1:N:348:ALA:O	1:N:349:LEU:HB2	2.01	0.60
1:S:404:GLU:H	1:S:404:GLU:CD	2.09	0.60
1:A:141:GLU:O	1:A:145:THR:OG1	2.18	0.60
1:J:151:TYR:HA	1:J:175:LEU:HD13	1.83	0.60
1:P:366:SER:O	1:P:367:LYS:HB2	1.99	0.60
1:H:3:LEU:HD23	1:H:3:LEU:O	2.02	0.60
1:C:424:LEU:O	1:C:427:SER:OG	2.19	0.60
1:H:174:CYS:O	1:H:178:VAL:HG23	2.02	0.60
1:M:29:ILE:O	1:M:33:GLU:HG3	2.01	0.60
1:A:190:LEU:HD11	1:A:194:PHE:CE2	2.37	0.60
1:A:408:THR:O	1:A:409:ASP:HB2	2.00	0.60
1:B:184:ILE:HD11	1:J:380:LEU:HB2	1.83	0.60
1:H:35:TYR:CD1	1:H:35:TYR:C	2.79	0.60
1:H:261:ILE:C	1:H:263:ASN:H	2.09	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:293:ALA:O	1:H:294:SER:HB3	2.01	0.60
1:K:414:THR:O	1:K:416:LEU:N	2.35	0.60
1:C:3:LEU:O	1:C:7:VAL:HG23	2.01	0.60
1:E:35:TYR:CD1	1:E:35:TYR:C	2.79	0.60
1:D:401:TYR:CZ	1:D:412:ARG:HG3	2.37	0.59
1:H:379:GLU:HG2	1:J:185:GLN:HG2	1.84	0.59
1:S:220:PRO:HB2	1:S:221:ARG:HG3	1.84	0.59
1:A:203:THR:C	1:A:206:PRO:HD2	2.25	0.59
1:D:235:LEU:O	1:D:239:GLU:HG3	2.02	0.59
1:I:64:ASN:OD1	1:I:65:ASN:N	2.34	0.59
1:J:7:VAL:O	1:J:11:TRP:HD1	1.85	0.59
1:A:51:ARG:HH21	1:A:92:GLU:CD	2.11	0.59
1:B:404:GLU:O	1:B:408:THR:HG22	2.02	0.59
1:J:89:ALA:O	1:J:93:TRP:HD1	1.86	0.59
1:D:203:THR:C	1:D:206:PRO:HD2	2.27	0.59
1:P:35:TYR:CD1	1:P:35:TYR:C	2.80	0.59
1:P:424:LEU:O	1:P:427:SER:OG	2.20	0.59
1:S:235:LEU:O	1:S:239:GLU:HG3	2.02	0.59
1:C:241:ASP:HA	1:C:299:VAL:HG13	1.84	0.59
1:C:278:ARG:HD2	1:C:374:TYR:CE1	2.37	0.59
1:M:408:THR:O	1:M:408:THR:OG1	2.18	0.59
1:N:283:ASP:C	1:N:283:ASP:OD1	2.45	0.59
1:G:35:TYR:CD1	1:G:35:TYR:C	2.79	0.59
1:H:28:LEU:HD12	1:H:28:LEU:O	2.03	0.59
1:O:13:VAL:HG13	1:O:14:LEU:HG	1.83	0.59
1:H:66:THR:O	1:H:70:ILE:HD12	2.02	0.59
1:M:242:THR:HB	1:M:301:HIS:HA	1.85	0.59
1:T:401:TYR:CZ	1:T:412:ARG:HG3	2.38	0.59
1:A:247:LEU:HD12	1:A:288:PHE:CE1	2.38	0.59
1:N:278:ARG:HD2	1:N:374:TYR:CE1	2.38	0.59
1:B:358:LEU:O	1:B:359:ARG:HB3	2.02	0.59
1:C:204:ARG:CZ	1:C:297:TRP:CZ2	2.85	0.59
1:D:220:PRO:HB2	1:D:221:ARG:HG3	1.85	0.59
1:A:102:LEU:O	1:A:171:THR:HG23	2.03	0.58
1:I:424:LEU:HD13	1:J:348:ALA:HB1	1.84	0.58
1:P:116:LYS:O	1:P:117:SER:C	2.46	0.58
1:Q:404:GLU:O	1:Q:408:THR:HG22	2.03	0.58
1:S:121:TYR:O	1:S:136:ARG:NH2	2.35	0.58
1:B:99:PHE:C	1:B:99:PHE:CD1	2.80	0.58
1:D:283:ASP:OD1	1:D:284:PRO:HD2	2.03	0.58
1:G:198:PHE:CE1	1:G:204:ARG:HG2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:75:VAL:O	1:N:79:VAL:HG13	2.02	0.58
1:O:430:ALA:O	1:O:431:VAL:HB	2.03	0.58
1:B:119:LEU:O	1:B:123:LEU:HD22	2.03	0.58
1:H:161:ASP:HA	1:H:164:SER:HA	1.85	0.58
1:L:99:PHE:CD1	1:L:99:PHE:C	2.81	0.58
1:L:299:VAL:HG12	1:L:300:PHE:N	2.18	0.58
1:S:208:LEU:O	1:S:209:SER:C	2.46	0.58
1:T:1:MSE:HE2	1:T:4:GLN:HB2	1.85	0.58
1:I:89:ALA:O	1:I:93:TRP:HD1	1.86	0.58
1:K:408:THR:O	1:K:409:ASP:HB2	2.03	0.58
1:L:426:ASN:N	1:L:426:ASN:OD1	2.36	0.58
1:E:220:PRO:HB2	1:E:221:ARG:HG3	1.85	0.58
1:L:293:ALA:O	1:L:294:SER:HB3	2.03	0.58
1:O:99:PHE:HB3	1:O:100:PRO:HD3	1.86	0.58
1:P:217:ARG:HG2	1:P:217:ARG:HH11	1.68	0.58
1:P:401:TYR:CZ	1:P:412:ARG:HG3	2.39	0.58
1:R:282:ILE:HD12	1:R:288:PHE:CE1	2.38	0.58
1:E:116:LYS:O	1:E:117:SER:C	2.47	0.58
1:H:80:ILE:HD12	1:H:93:TRP:CZ3	2.38	0.58
1:O:404:GLU:O	1:O:408:THR:HG23	2.03	0.58
1:E:85:LEU:O	1:E:135:LEU:HD22	2.03	0.58
1:E:293:ALA:O	1:E:294:SER:HB3	2.02	0.58
1:H:270:TYR:HB3	1:H:370:PHE:CE2	2.38	0.58
1:Q:150:LEU:O	1:Q:154:LYS:HB2	2.03	0.58
1:C:358:LEU:O	1:C:359:ARG:CB	2.50	0.57
1:M:62:PRO:HG2	1:M:64:ASN:CG	2.28	0.57
1:Q:72:TRP:O	1:Q:76:LEU:HD13	2.04	0.57
1:E:231:TYR:CE2	1:E:235:LEU:HD11	2.39	0.57
1:O:225:ILE:O	1:O:228:THR:OG1	2.22	0.57
1:S:71:LEU:O	1:S:75:VAL:HG23	2.04	0.57
1:C:24:ASP:N	1:C:26:THR:HG1	2.02	0.57
1:F:267:ASP:OD1	1:F:267:ASP:N	2.37	0.57
1:I:366:SER:O	1:I:367:LYS:HB2	2.05	0.57
1:T:79:VAL:C	1:T:81:PRO:HD2	2.30	0.57
1:H:150:LEU:O	1:H:154:LYS:HB2	2.05	0.57
1:G:142:GLU:OE2	1:G:146:ARG:NH1	2.38	0.57
1:H:144:ILE:O	1:H:148:VAL:HG23	2.05	0.57
1:H:185:GLN:O	1:H:221:ARG:NH2	2.38	0.57
1:C:99:PHE:CD1	1:C:99:PHE:C	2.83	0.57
1:D:50:ILE:O	1:D:54:LEU:HD22	2.05	0.57
1:D:203:THR:O	1:D:206:PRO:HD2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:76:LEU:HG	1:G:93:TRP:CZ3	2.39	0.57
1:H:129:ASP:O	1:H:131:TRP:N	2.38	0.57
1:R:7:VAL:HG13	1:R:53:ILE:HG21	1.87	0.57
1:A:150:LEU:O	1:A:154:LYS:HB2	2.05	0.57
1:A:247:LEU:HD12	1:A:288:PHE:CD1	2.40	0.57
1:I:115:LEU:HD22	1:I:119:LEU:HD22	1.86	0.57
1:I:278:ARG:HD2	1:I:374:TYR:CZ	2.40	0.57
1:J:36:GLN:HE21	1:J:36:GLN:HA	1.70	0.57
1:M:401:TYR:CZ	1:M:412:ARG:CG	2.84	0.57
1:F:89:ALA:O	1:F:92:GLU:HB2	2.05	0.57
1:K:205:ILE:HB	1:K:206:PRO:HD3	1.87	0.57
1:M:47:SER:O	1:M:51:ARG:HG3	2.05	0.56
1:O:408:THR:OG1	1:O:408:THR:O	2.17	0.56
1:A:269:LEU:HD22	1:A:273:PHE:CE1	2.39	0.56
1:E:180:VAL:O	1:E:184:ILE:HG23	2.05	0.56
1:G:86:ASP:HB3	1:G:135:LEU:CD2	2.36	0.56
1:H:293:ALA:O	1:H:294:SER:CB	2.53	0.56
1:M:150:LEU:O	1:M:154:LYS:HB2	2.04	0.56
1:M:360:ASP:CG	1:M:363:LEU:HB2	2.30	0.56
1:O:77:LYS:HD3	1:Q:292:THR:HG22	1.87	0.56
1:O:156:ILE:O	1:O:157:GLU:C	2.48	0.56
1:P:187:PRO:O	1:P:191:SER:OG	2.23	0.56
1:Q:231:TYR:CE2	1:Q:235:LEU:HD11	2.41	0.56
1:Q:273:PHE:HB3	1:Q:357:PHE:CE2	2.40	0.56
1:R:408:THR:O	1:R:409:ASP:HB2	2.05	0.56
1:S:115:LEU:HD22	1:S:119:LEU:HD22	1.85	0.56
1:B:86:ASP:HB3	1:B:135:LEU:HD22	1.87	0.56
1:H:148:VAL:O	1:H:152:VAL:HG23	2.06	0.56
1:O:366:SER:O	1:O:367:LYS:HB2	2.05	0.56
1:Q:409:ASP:C	1:Q:409:ASP:OD1	2.49	0.56
1:A:53:ILE:O	1:A:57:ILE:HG13	2.05	0.56
1:H:107:GLN:HE22	1:H:170:GLN:NE2	2.04	0.56
1:J:415:ARG:O	1:J:419:ILE:HG23	2.05	0.56
1:I:87:ARG:NH1	1:I:142:GLU:OE1	2.38	0.56
1:J:52:HIS:O	1:J:53:ILE:C	2.46	0.56
1:K:152:VAL:HG13	1:K:203:THR:HG22	1.85	0.56
1:O:35:TYR:CD1	1:O:35:TYR:C	2.84	0.56
1:O:47:SER:O	1:O:48:GLN:C	2.48	0.56
1:O:366:SER:O	1:O:367:LYS:CB	2.53	0.56
1:M:208:LEU:HD12	1:M:246:LEU:CD1	2.35	0.56
1:A:243:SER:O	1:A:244:PRO:C	2.47	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:180:VAL:O	1:D:184:ILE:HG23	2.05	0.56
1:F:151:TYR:HA	1:F:175:LEU:HD13	1.88	0.56
1:K:357:PHE:HD2	1:K:358:LEU:HD23	1.71	0.56
1:O:241:ASP:HA	1:O:299:VAL:HG13	1.87	0.56
1:G:215:ILE:HD11	1:G:253:PHE:CE2	2.41	0.56
1:O:185:GLN:O	1:O:221:ARG:NH2	2.38	0.55
1:P:83:LEU:N	1:P:83:LEU:HD23	2.20	0.55
1:C:217:ARG:HG2	1:C:217:ARG:HH11	1.72	0.55
1:L:396:SER:C	1:L:398:PHE:N	2.64	0.55
1:Q:154:LYS:HG2	1:Q:171:THR:HG21	1.88	0.55
1:A:164:SER:O	1:A:166:GLU:N	2.39	0.55
1:B:243:SER:OG	1:B:302:ASP:OD1	2.14	0.55
1:G:107:GLN:CD	1:G:170:GLN:HE22	2.14	0.55
1:R:365:ALA:HB1	1:R:370:PHE:O	2.06	0.55
1:S:148:VAL:HG21	1:S:193:CYS:HB3	1.88	0.55
1:K:32:VAL:HG13	1:K:82:LEU:HD21	1.87	0.55
1:L:203:THR:O	1:L:206:PRO:HD2	2.05	0.55
1:P:64:ASN:OD1	1:P:64:ASN:N	2.38	0.55
1:S:282:ILE:HD12	1:S:288:PHE:CZ	2.42	0.55
1:I:80:ILE:N	1:I:81:PRO:HD2	2.21	0.55
1:R:80:ILE:N	1:R:81:PRO:HD2	2.22	0.55
1:R:295:GLY:O	1:T:26:THR:HG23	2.06	0.55
1:A:250:ALA:O	1:A:254:ILE:HG23	2.07	0.55
1:M:132:GLY:O	1:M:135:LEU:HB2	2.07	0.55
1:M:280:SER:O	1:M:384:LYS:NZ	2.34	0.55
1:O:237:CYS:SG	1:O:246:LEU:HD21	2.47	0.55
1:P:366:SER:O	1:P:367:LYS:CB	2.55	0.55
1:E:223:TYR:CE2	1:F:414:THR:HG21	2.42	0.55
1:G:156:ILE:O	1:G:157:GLU:C	2.50	0.55
1:N:127:ASP:HB3	1:N:130:GLU:HB2	1.88	0.55
1:P:201:PRO:HB2	1:P:202:PRO:HD3	1.88	0.55
1:A:66:THR:O	1:A:69:ARG:N	2.39	0.55
1:A:360:ASP:CG	1:A:363:LEU:HB2	2.32	0.55
1:N:50:ILE:O	1:N:54:LEU:HD22	2.06	0.55
1:T:174:CYS:O	1:T:178:VAL:HG23	2.06	0.55
1:H:8:LYS:HG2	1:H:12:ASN:HD21	1.72	0.55
1:J:430:ALA:O	1:J:431:VAL:HB	2.07	0.55
1:O:199:LEU:O	1:O:201:PRO:HD3	2.06	0.55
1:Q:250:ALA:O	1:Q:254:ILE:HG23	2.07	0.55
1:R:242:THR:HG21	1:T:110:PRO:HG3	1.89	0.55
1:T:71:LEU:O	1:T:75:VAL:HG23	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:TYR:C	1:A:35:TYR:CD1	2.85	0.55
1:O:121:TYR:O	1:O:136:ARG:NH2	2.40	0.55
1:I:189:GLU:OE1	1:I:189:GLU:N	2.39	0.54
1:M:185:GLN:HA	1:O:379:GLU:CG	2.32	0.54
1:R:278:ARG:HD2	1:R:374:TYR:CZ	2.41	0.54
1:T:366:SER:O	1:T:367:LYS:HB2	2.07	0.54
1:A:165:GLN:O	1:A:168:ARG:N	2.40	0.54
1:G:414:THR:HG21	1:H:223:TYR:CD2	2.42	0.54
1:I:417:ASP:O	1:I:421:VAL:HG23	2.06	0.54
1:L:152:VAL:HG13	1:L:203:THR:HG22	1.89	0.54
1:N:1:MSE:HE2	1:N:4:GLN:HB2	1.89	0.54
1:Q:261:ILE:HG22	1:Q:263:ASN:H	1.72	0.54
1:Q:366:SER:O	1:Q:367:LYS:HB2	2.06	0.54
1:S:69:ARG:NH1	1:S:104:SER:O	2.38	0.54
1:S:152:VAL:CG1	1:S:203:THR:HG22	2.37	0.54
1:F:269:LEU:HD11	1:F:350:TYR:CD1	2.41	0.54
1:H:107:GLN:HE22	1:H:170:GLN:HE22	1.53	0.54
1:M:282:ILE:HD12	1:M:288:PHE:CZ	2.43	0.54
1:D:261:ILE:HG22	1:D:262:CYS:N	2.22	0.54
1:L:151:TYR:HA	1:L:175:LEU:HD13	1.89	0.54
1:M:62:PRO:HG2	1:M:64:ASN:ND2	2.23	0.54
1:B:25:LEU:HD21	1:B:74:ALA:HB1	1.89	0.54
1:D:280:SER:O	1:D:281:MSE:HE2	2.08	0.54
1:A:80:ILE:N	1:A:81:PRO:HD2	2.23	0.54
1:E:13:VAL:HG11	1:E:28:LEU:HD22	1.88	0.54
1:N:379:GLU:HG3	1:P:185:GLN:HA	1.90	0.54
1:S:47:SER:O	1:S:51:ARG:HG3	2.06	0.54
1:T:405:THR:O	1:T:409:ASP:HB2	2.08	0.54
1:D:231:TYR:CZ	1:D:235:LEU:HD11	2.43	0.54
1:E:121:TYR:O	1:E:136:ARG:NH2	2.40	0.54
1:F:80:ILE:N	1:F:81:PRO:HD2	2.22	0.54
1:L:247:LEU:HD12	1:L:288:PHE:CE1	2.42	0.54
1:S:201:PRO:HB2	1:S:202:PRO:HD3	1.89	0.54
1:G:250:ALA:O	1:G:254:ILE:HG23	2.08	0.54
1:M:6:LEU:O	1:M:9:ALA:HB3	2.08	0.54
1:N:217:ARG:HG2	1:N:217:ARG:HH11	1.73	0.54
1:N:260:HIS:C	1:N:261:ILE:HG13	2.33	0.54
1:P:121:TYR:O	1:P:136:ARG:NH2	2.41	0.54
1:Q:430:ALA:HB3	1:R:391:ARG:O	2.07	0.54
1:M:416:LEU:HG	1:N:420:ALA:HB1	1.90	0.54
1:N:53:ILE:O	1:N:57:ILE:HG13	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:203:THR:C	1:N:206:PRO:HD2	2.33	0.54
1:S:180:VAL:HG12	1:S:181:HIS:N	2.22	0.54
1:D:65:ASN:ND2	1:D:68:ARG:HG3	2.22	0.54
1:J:201:PRO:HB2	1:J:202:PRO:HD3	1.89	0.54
1:K:349:LEU:O	1:K:412:ARG:NH1	2.39	0.54
1:P:86:ASP:HB3	1:P:135:LEU:HD22	1.90	0.54
1:B:250:ALA:O	1:B:254:ILE:HG23	2.07	0.53
1:G:356:GLU:HG3	1:G:359:ARG:NH2	2.23	0.53
1:H:208:LEU:O	1:H:211:MSE:N	2.40	0.53
1:M:191:SER:HB2	1:M:228:THR:HG21	1.91	0.53
1:S:129:ASP:O	1:S:131:TRP:N	2.42	0.53
1:C:71:LEU:O	1:C:75:VAL:HG23	2.08	0.53
1:N:80:ILE:N	1:N:81:PRO:HD2	2.21	0.53
1:S:267:ASP:OD1	1:S:267:ASP:N	2.41	0.53
1:D:343:PHE:CD1	1:D:343:PHE:C	2.87	0.53
1:M:85:LEU:O	1:M:135:LEU:HD22	2.07	0.53
1:M:217:ARG:O	1:M:218:GLN:C	2.50	0.53
1:O:176:VAL:HG12	1:O:177:ASN:N	2.23	0.53
1:C:215:ILE:HD13	1:C:222:LEU:HD22	1.89	0.53
1:G:262:CYS:HA	1:G:265:LEU:HD12	1.91	0.53
1:I:242:THR:HG22	1:I:301:HIS:HA	1.90	0.53
1:N:241:ASP:HA	1:N:299:VAL:HG13	1.90	0.53
1:R:28:LEU:O	1:R:32:VAL:HG23	2.07	0.53
1:F:107:GLN:O	1:F:108:LEU:HD23	2.08	0.53
1:N:254:ILE:HD11	1:N:272:LEU:CD2	2.38	0.53
1:P:237:CYS:SG	1:P:246:LEU:HD21	2.49	0.53
1:S:293:ALA:O	1:S:294:SER:HB3	2.08	0.53
1:B:3:LEU:O	1:B:7:VAL:HG23	2.08	0.53
1:I:349:LEU:O	1:I:412:ARG:NH1	2.38	0.53
1:L:204:ARG:CZ	1:L:297:TRP:CZ2	2.92	0.53
1:S:402:THR:OG1	1:S:405:THR:HG23	2.08	0.53
1:M:231:TYR:CZ	1:M:235:LEU:HD11	2.44	0.53
1:C:299:VAL:O	1:C:304:MSE:HE1	2.09	0.53
1:D:32:VAL:HG13	1:D:82:LEU:HD11	1.90	0.53
1:J:89:ALA:O	1:J:93:TRP:CD1	2.61	0.53
1:O:1:MSE:HE1	1:O:8:LYS:NZ	2.23	0.53
1:R:293:ALA:CB	1:R:373:ARG:HE	2.20	0.53
1:B:292:THR:HG22	1:D:77:LYS:HD3	1.91	0.53
1:F:115:LEU:HD22	1:F:119:LEU:HD22	1.89	0.53
1:F:366:SER:O	1:F:367:LYS:HB2	2.07	0.53
1:H:47:SER:O	1:H:51:ARG:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:254:ILE:O	1:L:258:LEU:HB2	2.09	0.53
1:M:251:LEU:O	1:M:254:ILE:N	2.41	0.53
1:Q:148:VAL:HG21	1:Q:193:CYS:SG	2.49	0.53
1:F:386:ASP:O	1:F:388:LEU:N	2.42	0.53
1:G:79:VAL:C	1:G:81:PRO:HD2	2.34	0.53
1:M:401:TYR:CE1	1:M:412:ARG:HG3	2.41	0.53
1:N:267:ASP:OD1	1:N:267:ASP:N	2.42	0.53
1:P:404:GLU:O	1:P:408:THR:HG22	2.08	0.53
1:Q:410:LYS:C	1:Q:412:ARG:H	2.16	0.53
1:I:204:ARG:HB3	1:I:246:LEU:HD11	1.90	0.52
1:K:142:GLU:HG3	1:K:146:ARG:HD2	1.91	0.52
1:L:396:SER:O	1:L:397:ASN:C	2.52	0.52
1:O:99:PHE:CE1	1:O:103:ASN:OD1	2.62	0.52
1:Q:79:VAL:C	1:Q:81:PRO:HD2	2.34	0.52
1:R:401:TYR:CE2	1:R:412:ARG:HG3	2.44	0.52
1:K:10:LEU:O	1:K:14:LEU:HD12	2.09	0.52
1:K:243:SER:OG	1:K:302:ASP:CG	2.52	0.52
1:A:115:LEU:HD22	1:A:119:LEU:HD22	1.91	0.52
1:B:2:PRO:HG3	1:B:38:ARG:CD	2.39	0.52
1:B:255:LEU:HD23	1:B:337:LEU:HB3	1.91	0.52
1:D:242:THR:HB	1:D:301:HIS:HA	1.92	0.52
1:E:402:THR:O	1:E:403:ALA:C	2.51	0.52
1:G:1:MSE:HE2	1:G:4:GLN:HB3	1.90	0.52
1:G:121:TYR:O	1:G:136:ARG:NH2	2.42	0.52
1:G:229:GLY:O	1:G:233:LEU:HD13	2.09	0.52
1:K:393:LEU:HB2	1:L:428:LEU:HD12	1.91	0.52
1:L:99:PHE:HB3	1:L:100:PRO:HD3	1.91	0.52
1:A:242:THR:HG21	1:I:110:PRO:HG2	1.91	0.52
1:E:366:SER:O	1:E:367:LYS:CB	2.57	0.52
1:H:145:THR:O	1:H:149:ASP:OD1	2.26	0.52
1:K:235:LEU:O	1:K:239:GLU:HG3	2.09	0.52
1:M:208:LEU:HD12	1:M:246:LEU:HD12	1.92	0.52
1:Q:76:LEU:O	1:Q:80:ILE:HG22	2.09	0.52
1:R:35:TYR:CE1	1:R:82:LEU:HG	2.44	0.52
1:K:408:THR:O	1:K:409:ASP:CB	2.58	0.52
1:Q:65:ASN:ND2	1:Q:68:ARG:HG3	2.25	0.52
1:S:282:ILE:HD12	1:S:288:PHE:CE1	2.44	0.52
1:D:154:LYS:HG2	1:D:171:THR:HG21	1.90	0.52
1:H:239:GLU:OE2	1:H:271:ARG:NH2	2.43	0.52
1:L:293:ALA:O	1:L:294:SER:CB	2.58	0.52
1:O:420:ALA:HB2	1:P:420:ALA:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:201:PRO:HB2	1:Q:202:PRO:HD3	1.91	0.52
1:B:2:PRO:HG3	1:B:38:ARG:HD2	1.91	0.52
1:L:99:PHE:HB3	1:L:100:PRO:CD	2.40	0.52
1:E:278:ARG:HD2	1:E:374:TYR:CZ	2.44	0.52
1:K:366:SER:O	1:K:367:LYS:HB2	2.09	0.52
1:Q:94:TRP:CD1	1:Q:146:ARG:HE	2.28	0.52
1:Q:241:ASP:OD1	1:Q:297:TRP:NE1	2.32	0.52
1:T:53:ILE:O	1:T:57:ILE:HG13	2.10	0.52
1:D:277:LEU:C	1:D:277:LEU:CD2	2.83	0.52
1:F:354:PHE:CZ	1:F:358:LEU:HD11	2.45	0.52
1:K:180:VAL:HG13	1:K:214:VAL:CG2	2.38	0.52
1:L:379:GLU:HG2	1:N:185:GLN:HG2	1.90	0.52
1:L:380:LEU:HB2	1:N:184:ILE:HD11	1.92	0.52
1:Q:171:THR:HG22	1:Q:175:LEU:HD12	1.92	0.52
1:Q:217:ARG:HG2	1:Q:217:ARG:HH11	1.74	0.52
1:S:241:ASP:HA	1:S:299:VAL:HG13	1.92	0.52
1:B:150:LEU:HG	1:B:175:LEU:HD11	1.91	0.52
1:C:396:SER:O	1:C:398:PHE:N	2.43	0.52
1:J:141:GLU:O	1:J:145:THR:OG1	2.26	0.52
1:K:242:THR:HG21	1:S:110:PRO:HG3	1.91	0.52
1:M:35:TYR:CD1	1:M:35:TYR:C	2.87	0.52
1:R:292:THR:HG23	1:R:373:ARG:O	2.09	0.52
1:S:35:TYR:CD1	1:S:35:TYR:C	2.87	0.52
1:C:299:VAL:HG11	1:C:301:HIS:CE1	2.45	0.51
1:H:349:LEU:O	1:H:412:ARG:NH1	2.34	0.51
1:I:99:PHE:CD1	1:I:99:PHE:C	2.87	0.51
1:G:32:VAL:O	1:G:33:GLU:C	2.53	0.51
1:L:382:SER:O	1:L:383:THR:C	2.53	0.51
1:P:99:PHE:HB3	1:P:100:PRO:HD3	1.92	0.51
1:P:102:LEU:O	1:P:171:THR:HG23	2.10	0.51
1:T:32:VAL:O	1:T:36:GLN:HG2	2.10	0.51
1:A:10:LEU:O	1:A:14:LEU:HD12	2.09	0.51
1:D:292:THR:HG22	1:F:77:LYS:HD3	1.92	0.51
1:J:83:LEU:N	1:J:83:LEU:HD23	2.24	0.51
1:C:366:SER:O	1:C:367:LYS:CB	2.58	0.51
1:C:382:SER:O	1:C:383:THR:C	2.52	0.51
1:D:277:LEU:HD23	1:D:277:LEU:O	2.10	0.51
1:E:151:TYR:HA	1:E:175:LEU:HD13	1.93	0.51
1:I:247:LEU:HD12	1:I:288:PHE:CD1	2.45	0.51
1:K:357:PHE:CD2	1:K:358:LEU:HD23	2.45	0.51
1:M:13:VAL:HG13	1:M:14:LEU:HG	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:130:GLU:OE1	1:Q:136:ARG:NH1	2.43	0.51
1:R:32:VAL:HG13	1:R:82:LEU:HD21	1.91	0.51
1:R:261:ILE:C	1:R:263:ASN:H	2.18	0.51
1:C:401:TYR:CZ	1:C:412:ARG:HG3	2.46	0.51
1:O:99:PHE:CD1	1:O:99:PHE:C	2.89	0.51
1:Q:345:ILE:O	1:Q:345:ILE:HG13	2.10	0.51
1:Q:366:SER:C	1:Q:368:HIS:H	2.19	0.51
1:R:261:ILE:O	1:R:263:ASN:N	2.39	0.51
1:R:292:THR:OG1	1:R:293:ALA:N	2.43	0.51
1:A:297:TRP:O	1:A:298:GLU:CB	2.58	0.51
1:R:65:ASN:C	1:R:65:ASN:OD1	2.54	0.51
1:C:401:TYR:CE2	1:C:412:ARG:HG3	2.46	0.51
1:F:47:SER:O	1:F:51:ARG:HG3	2.11	0.51
1:I:121:TYR:O	1:I:136:ARG:NH2	2.44	0.51
1:N:366:SER:O	1:N:367:LYS:HB2	2.10	0.51
1:Q:43:ASN:HB3	1:Q:46:ASN:HB2	1.92	0.51
1:D:130:GLU:OE1	1:D:136:ARG:NH1	2.43	0.51
1:D:283:ASP:OD1	1:D:283:ASP:C	2.53	0.51
1:F:79:VAL:C	1:F:81:PRO:HD2	2.35	0.51
1:H:190:LEU:HD11	1:H:194:PHE:CE2	2.46	0.51
1:L:46:ASN:O	1:L:50:ILE:HG13	2.11	0.51
1:M:53:ILE:O	1:M:56:GLU:HB2	2.10	0.51
1:M:230:PHE:O	1:M:234:VAL:HG23	2.10	0.51
1:M:250:ALA:O	1:M:254:ILE:HG23	2.11	0.51
1:O:261:ILE:HG21	1:O:264:SER:HB2	1.93	0.51
1:O:291:SER:OG	1:O:292:THR:N	2.43	0.51
1:S:402:THR:H	1:S:405:THR:HG1	1.58	0.51
1:T:65:ASN:C	1:T:65:ASN:OD1	2.54	0.51
1:B:205:ILE:HB	1:B:206:PRO:HD3	1.93	0.51
1:I:131:TRP:CE3	1:I:136:ARG:HD2	2.46	0.51
1:L:261:ILE:O	1:L:263:ASN:N	2.43	0.51
1:M:366:SER:O	1:M:367:LYS:HB2	2.10	0.51
1:N:406:GLU:O	1:N:412:ARG:NH2	2.42	0.51
1:Q:401:TYR:CZ	1:Q:412:ARG:HG3	2.46	0.51
1:C:401:TYR:OH	1:C:412:ARG:HG3	2.11	0.51
1:F:198:PHE:CE1	1:F:204:ARG:HG2	2.46	0.51
1:F:210:VAL:O	1:F:214:VAL:HG23	2.10	0.51
1:J:51:ARG:NH2	1:J:92:GLU:OE2	2.37	0.51
1:J:242:THR:O	1:J:244:PRO:HD3	2.09	0.51
1:S:144:ILE:O	1:S:148:VAL:HG23	2.10	0.51
1:S:201:PRO:O	1:S:202:PRO:C	2.52	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:297:TRP:O	1:C:298:GLU:HB3	2.11	0.50
1:E:80:ILE:N	1:E:81:PRO:CD	2.74	0.50
1:F:27:GLU:O	1:F:30:ALA:HB3	2.11	0.50
1:F:152:VAL:HG13	1:F:203:THR:HG22	1.93	0.50
1:G:80:ILE:N	1:G:81:PRO:CD	2.74	0.50
1:J:99:PHE:C	1:J:99:PHE:CD1	2.89	0.50
1:N:203:THR:O	1:N:206:PRO:HD2	2.10	0.50
1:O:260:HIS:C	1:O:261:ILE:HG13	2.36	0.50
1:Q:65:ASN:OD1	1:Q:66:THR:N	2.44	0.50
1:B:63:PHE:CE1	1:B:69:ARG:HA	2.46	0.50
1:M:1:MSE:HE2	1:M:4:GLN:HB2	1.93	0.50
1:S:65:ASN:ND2	1:S:68:ARG:HG3	2.26	0.50
1:A:292:THR:HG23	1:A:373:ARG:O	2.11	0.50
1:F:1:MSE:HE2	1:F:4:GLN:HB2	1.92	0.50
1:F:215:ILE:HD13	1:F:222:LEU:HD22	1.94	0.50
1:G:215:ILE:O	1:G:216:ARG:C	2.55	0.50
1:I:201:PRO:O	1:I:202:PRO:C	2.54	0.50
1:K:294:SER:O	1:K:295:GLY:C	2.55	0.50
1:P:247:LEU:HD12	1:P:288:PHE:CE1	2.45	0.50
1:R:366:SER:O	1:R:367:LYS:CB	2.58	0.50
1:T:3:LEU:O	1:T:3:LEU:HD23	2.11	0.50
1:A:396:SER:O	1:A:398:PHE:N	2.44	0.50
1:E:278:ARG:HD2	1:E:374:TYR:CE1	2.46	0.50
1:L:186:ARG:HB3	1:L:189:GLU:OE1	2.12	0.50
1:O:282:ILE:HD12	1:O:288:PHE:CZ	2.47	0.50
1:A:153:SER:O	1:A:157:GLU:HG2	2.12	0.50
1:G:278:ARG:HD2	1:G:374:TYR:CE1	2.47	0.50
1:M:51:ARG:NH2	1:M:92:GLU:OE1	2.44	0.50
1:N:269:LEU:HD22	1:N:273:PHE:CE1	2.47	0.50
1:Q:351:PRO:O	1:Q:352:ILE:C	2.53	0.50
1:S:268:SER:O	1:S:269:LEU:C	2.55	0.50
1:A:327:GLY:O	1:A:328:SER:CB	2.59	0.50
1:B:291:SER:OG	1:B:292:THR:N	2.45	0.50
1:F:144:ILE:O	1:F:148:VAL:HG23	2.12	0.50
1:G:1:MSE:HE2	1:G:4:GLN:CB	2.41	0.50
1:K:80:ILE:N	1:K:81:PRO:HD2	2.27	0.50
1:A:243:SER:HB3	1:A:246:LEU:HB3	1.92	0.50
1:A:401:TYR:CE2	1:A:412:ARG:HG3	2.47	0.50
1:H:379:GLU:HG3	1:J:185:GLN:HA	1.94	0.50
1:J:210:VAL:O	1:J:214:VAL:HG23	2.10	0.50
1:Q:80:ILE:N	1:Q:81:PRO:HD2	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:109:LYS:N	1:S:110:PRO:CD	2.75	0.50
1:C:151:TYR:HB2	1:C:175:LEU:HD13	1.92	0.50
1:E:205:ILE:HB	1:E:206:PRO:HD3	1.93	0.50
1:F:243:SER:HB3	1:F:246:LEU:HB3	1.93	0.50
1:H:99:PHE:CD1	1:H:99:PHE:C	2.89	0.50
1:N:401:TYR:CZ	1:N:412:ARG:HG3	2.47	0.50
1:O:215:ILE:CG2	1:O:256:MSE:HB3	2.41	0.50
1:A:71:LEU:O	1:A:75:VAL:HG23	2.12	0.50
1:A:293:ALA:O	1:A:294:SER:HB3	2.11	0.50
1:B:151:TYR:CA	1:B:175:LEU:HD13	2.42	0.50
1:H:80:ILE:N	1:H:81:PRO:HD2	2.27	0.50
1:H:176:VAL:HG13	1:H:210:VAL:HG22	1.93	0.50
1:H:300:PHE:CD1	1:H:301:HIS:O	2.64	0.50
1:M:119:LEU:O	1:M:123:LEU:HD22	2.11	0.50
1:O:409:ASP:OD1	1:O:409:ASP:C	2.54	0.50
1:Q:348:ALA:O	1:Q:349:LEU:HB2	2.12	0.50
1:B:402:THR:OG1	1:B:404:GLU:HG2	2.11	0.49
1:D:71:LEU:O	1:D:72:TRP:C	2.55	0.49
1:E:32:VAL:O	1:E:36:GLN:HG3	2.11	0.49
1:F:205:ILE:HB	1:F:206:PRO:HD3	1.92	0.49
1:I:343:PHE:C	1:I:343:PHE:CD1	2.90	0.49
1:K:151:TYR:HA	1:K:175:LEU:HD13	1.94	0.49
1:K:201:PRO:HB3	1:K:300:PHE:HB2	1.94	0.49
1:N:205:ILE:HB	1:N:206:PRO:HD3	1.94	0.49
1:Q:204:ARG:CZ	1:Q:297:TRP:CZ2	2.94	0.49
1:S:54:LEU:HD12	1:S:72:TRP:HZ3	1.76	0.49
1:S:119:LEU:O	1:S:123:LEU:HD22	2.12	0.49
1:A:1:MSE:HE2	1:A:4:GLN:HB2	1.93	0.49
1:A:184:ILE:HD11	1:C:380:LEU:HB2	1.94	0.49
1:G:76:LEU:HG	1:G:93:TRP:CH2	2.47	0.49
1:H:14:LEU:HD13	1:H:57:ILE:HG21	1.93	0.49
1:J:80:ILE:N	1:J:81:PRO:HD2	2.27	0.49
1:K:71:LEU:O	1:K:75:VAL:HG23	2.12	0.49
1:K:241:ASP:HA	1:K:299:VAL:HG13	1.93	0.49
1:N:46:ASN:O	1:N:50:ILE:HG13	2.12	0.49
1:N:131:TRP:O	1:N:135:LEU:HD12	2.11	0.49
1:O:80:ILE:N	1:O:81:PRO:CD	2.74	0.49
1:O:217:ARG:HG2	1:O:217:ARG:HH11	1.75	0.49
1:R:251:LEU:HD22	1:R:255:LEU:HD13	1.95	0.49
1:R:349:LEU:O	1:R:412:ARG:NH1	2.43	0.49
1:T:409:ASP:OD1	1:T:411:SER:OG	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:297:TRP:O	1:C:298:GLU:CB	2.59	0.49
1:G:177:ASN:C	1:G:177:ASN:OD1	2.54	0.49
1:G:243:SER:HB3	1:G:246:LEU:HB3	1.93	0.49
1:H:268:SER:O	1:H:269:LEU:C	2.56	0.49
1:I:414:THR:HG21	1:J:223:TYR:CD2	2.47	0.49
1:J:3:LEU:O	1:J:3:LEU:HD23	2.12	0.49
1:J:243:SER:HB3	1:J:246:LEU:HB3	1.93	0.49
1:K:204:ARG:HB3	1:K:246:LEU:HD11	1.94	0.49
1:L:210:VAL:O	1:L:211:MSE:C	2.54	0.49
1:L:273:PHE:HB3	1:L:357:PHE:CZ	2.47	0.49
1:M:263:ASN:C	1:M:265:LEU:H	2.20	0.49
1:B:25:LEU:O	1:B:26:THR:C	2.56	0.49
1:B:148:VAL:HG21	1:B:193:CYS:CB	2.42	0.49
1:K:208:LEU:O	1:K:212:VAL:HG13	2.12	0.49
1:L:65:ASN:C	1:L:65:ASN:OD1	2.54	0.49
1:L:187:PRO:O	1:L:188:LYS:C	2.54	0.49
1:P:108:LEU:HB3	1:P:111:VAL:HG23	1.93	0.49
1:T:269:LEU:HD22	1:T:273:PHE:CE1	2.46	0.49
1:A:106:THR:HG22	1:A:108:LEU:HB2	1.95	0.49
1:C:80:ILE:N	1:C:81:PRO:HD2	2.27	0.49
1:C:110:PRO:HG3	1:E:242:THR:HG21	1.94	0.49
1:D:115:LEU:O	1:D:115:LEU:HD22	2.13	0.49
1:D:409:ASP:OD1	1:D:411:SER:OG	2.27	0.49
1:F:175:LEU:O	1:F:179:LEU:HD12	2.13	0.49
1:H:65:ASN:ND2	1:H:68:ARG:HG3	2.28	0.49
1:K:366:SER:O	1:K:367:LYS:CB	2.60	0.49
1:P:84:ILE:C	1:P:85:LEU:HD12	2.36	0.49
1:S:201:PRO:HB2	1:S:202:PRO:CD	2.41	0.49
1:A:176:VAL:O	1:A:177:ASN:C	2.55	0.49
1:C:236:LYS:O	1:C:237:CYS:C	2.56	0.49
1:D:366:SER:O	1:D:367:LYS:HB2	2.12	0.49
1:E:29:ILE:HG22	1:E:33:GLU:OE2	2.13	0.49
1:G:1:MSE:N	1:G:2:PRO:HD3	2.27	0.49
1:H:81:PRO:HA	1:H:121:TYR:CZ	2.47	0.49
1:L:1:MSE:HE2	1:L:4:GLN:CB	2.41	0.49
1:L:235:LEU:O	1:L:239:GLU:HG3	2.13	0.49
1:O:289:PRO:HB3	1:O:374:TYR:HB3	1.94	0.49
1:P:1:MSE:HG2	1:P:4:GLN:HG3	1.93	0.49
1:R:64:ASN:OD1	1:R:68:ARG:NH1	2.44	0.49
1:S:7:VAL:HG13	1:S:53:ILE:HG21	1.94	0.49
1:S:289:PRO:HB2	1:S:374:TYR:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:91:GLY:O	1:T:95:ASP:OD2	2.31	0.49
1:E:294:SER:O	1:E:295:GLY:C	2.54	0.49
1:E:430:ALA:O	1:E:431:VAL:HB	2.12	0.49
1:F:304:MSE:O	1:F:305:SER:CB	2.61	0.49
1:M:185:GLN:O	1:M:221:ARG:NH2	2.46	0.49
1:Q:161:ASP:HA	1:Q:164:SER:CB	2.43	0.49
1:C:347:TYR:O	1:C:351:PRO:HB3	2.12	0.49
1:F:299:VAL:O	1:F:304:MSE:HE1	2.13	0.49
1:P:99:PHE:CE1	1:P:103:ASN:HB2	2.47	0.49
1:P:241:ASP:O	1:P:278:ARG:NH2	2.41	0.49
1:R:225:ILE:HB	1:R:226:PRO:HD3	1.95	0.49
1:S:200:ASN:O	1:S:203:THR:OG1	2.11	0.49
1:T:99:PHE:HB3	1:T:100:PRO:HD3	1.93	0.49
1:T:190:LEU:HD11	1:T:194:PHE:CE2	2.48	0.49
1:E:223:TYR:O	1:E:226:PRO:HD2	2.13	0.49
1:J:267:ASP:N	1:J:267:ASP:OD1	2.45	0.49
1:P:351:PRO:HG3	1:P:395:HIS:CE1	2.48	0.49
1:S:201:PRO:HB3	1:S:300:PHE:HB2	1.93	0.49
1:A:276:TYR:HB2	1:A:342:LEU:HD23	1.95	0.49
1:D:135:LEU:O	1:D:136:ARG:C	2.54	0.49
1:J:151:TYR:CE1	1:J:176:VAL:HG23	2.48	0.49
1:J:351:PRO:HD2	1:J:406:GLU:OE2	2.12	0.49
1:O:14:LEU:HA	1:O:71:LEU:HD21	1.94	0.49
1:O:42:GLN:NE2	1:O:81:PRO:O	2.45	0.49
1:S:205:ILE:HB	1:S:206:PRO:CD	2.42	0.49
1:T:62:PRO:HG2	1:T:64:ASN:ND2	2.28	0.49
1:J:53:ILE:O	1:J:57:ILE:HG13	2.13	0.48
1:J:241:ASP:HA	1:J:299:VAL:HG13	1.95	0.48
1:L:38:ARG:HD3	1:L:39:TYR:CZ	2.48	0.48
1:M:406:GLU:O	1:M:412:ARG:NH2	2.44	0.48
1:R:408:THR:O	1:R:409:ASP:CB	2.60	0.48
1:S:118:ILE:O	1:S:119:LEU:C	2.56	0.48
1:C:14:LEU:HD13	1:C:57:ILE:HG21	1.94	0.48
1:C:396:SER:O	1:C:397:ASN:C	2.57	0.48
1:E:84:ILE:O	1:E:85:LEU:HD12	2.13	0.48
1:I:196:HIS:CD2	1:I:197:HIS:CD2	3.00	0.48
1:I:255:LEU:HD21	1:I:341:GLN:HB3	1.94	0.48
1:K:401:TYR:CZ	1:K:412:ARG:HG3	2.48	0.48
1:L:94:TRP:CD1	1:L:146:ARG:HE	2.32	0.48
1:N:237:CYS:SG	1:N:246:LEU:HD11	2.53	0.48
1:S:205:ILE:HG22	1:S:206:PRO:HD3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:121:TYR:O	1:T:136:ARG:NH2	2.45	0.48
1:G:35:TYR:CE1	1:G:39:TYR:HB2	2.49	0.48
1:G:99:PHE:CD1	1:G:99:PHE:C	2.92	0.48
1:H:209:SER:HA	1:H:249:TYR:CE1	2.49	0.48
1:J:129:ASP:O	1:J:132:GLY:N	2.43	0.48
1:K:414:THR:HG21	1:L:223:TYR:CE2	2.48	0.48
1:M:409:ASP:OD1	1:M:411:SER:OG	2.21	0.48
1:S:293:ALA:O	1:S:294:SER:CB	2.62	0.48
1:T:414:THR:O	1:T:416:LEU:N	2.47	0.48
1:A:211:MSE:O	1:A:215:ILE:HG12	2.14	0.48
1:B:151:TYR:HA	1:B:175:LEU:HD13	1.96	0.48
1:J:347:TYR:O	1:J:351:PRO:HB3	2.13	0.48
1:K:94:TRP:CG	1:K:146:ARG:HE	2.31	0.48
1:N:352:ILE:HG21	1:N:403:ALA:HA	1.95	0.48
1:R:209:SER:HA	1:R:249:TYR:CE1	2.48	0.48
1:S:151:TYR:CA	1:S:175:LEU:HD13	2.41	0.48
1:B:347:TYR:O	1:B:351:PRO:HB3	2.13	0.48
1:F:231:TYR:CZ	1:F:235:LEU:HD11	2.49	0.48
1:I:255:LEU:HD23	1:I:337:LEU:HB3	1.96	0.48
1:T:52:HIS:O	1:T:56:GLU:HG2	2.12	0.48
1:B:430:ALA:O	1:B:431:VAL:HB	2.13	0.48
1:J:76:LEU:O	1:J:77:LYS:C	2.56	0.48
1:N:99:PHE:HB3	1:N:100:PRO:CD	2.43	0.48
1:T:414:THR:C	1:T:416:LEU:N	2.71	0.48
1:B:293:ALA:HB3	1:B:373:ARG:HE	1.77	0.48
1:B:349:LEU:O	1:B:412:ARG:NH1	2.46	0.48
1:E:276:TYR:O	1:E:277:LEU:C	2.55	0.48
1:G:142:GLU:O	1:G:146:ARG:HG3	2.14	0.48
1:H:269:LEU:HD22	1:H:273:PHE:CE1	2.49	0.48
1:N:35:TYR:HE2	1:N:46:ASN:HD22	1.62	0.48
1:N:404:GLU:O	1:N:408:THR:HG22	2.14	0.48
1:O:63:PHE:CE1	1:O:69:ARG:HA	2.48	0.48
1:P:63:PHE:CE2	1:P:69:ARG:HG2	2.49	0.48
1:P:226:PRO:HG3	1:P:261:ILE:HD11	1.95	0.48
1:P:241:ASP:HA	1:P:299:VAL:HG13	1.95	0.48
1:S:366:SER:O	1:S:367:LYS:CB	2.61	0.48
1:C:267:ASP:OD1	1:C:267:ASP:N	2.47	0.48
1:F:121:TYR:O	1:F:136:ARG:NH2	2.46	0.48
1:G:299:VAL:O	1:G:304:MSE:HE1	2.13	0.48
1:H:292:THR:HG22	1:J:77:LYS:HE2	1.95	0.48
1:I:65:ASN:C	1:I:65:ASN:OD1	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:35:TYR:CD1	1:J:35:TYR:C	2.91	0.48
1:J:353:ASN:HD21	1:J:407:LEU:HG	1.78	0.48
1:J:366:SER:O	1:J:367:LYS:CB	2.61	0.48
1:O:222:LEU:O	1:O:223:TYR:C	2.55	0.48
1:P:80:ILE:N	1:P:81:PRO:CD	2.77	0.48
1:S:3:LEU:HD23	1:S:3:LEU:O	2.14	0.48
1:T:32:VAL:HG13	1:T:82:LEU:HD21	1.95	0.48
1:A:67:ARG:HA	1:A:70:ILE:HD12	1.96	0.48
1:A:185:GLN:HA	1:C:379:GLU:HG3	1.96	0.48
1:C:121:TYR:O	1:C:136:ARG:NH2	2.45	0.48
1:E:113:SER:O	1:E:117:SER:HB2	2.14	0.48
1:J:116:LYS:O	1:J:117:SER:C	2.57	0.48
1:J:268:SER:O	1:J:269:LEU:C	2.57	0.48
1:L:341:GLN:O	1:L:345:ILE:HG22	2.14	0.48
1:N:189:GLU:O	1:N:190:LEU:C	2.56	0.48
1:N:297:TRP:O	1:N:298:GLU:CB	2.61	0.48
1:P:99:PHE:N	1:P:100:PRO:CD	2.77	0.48
1:P:430:ALA:O	1:P:431:VAL:CB	2.62	0.48
1:S:54:LEU:HD12	1:S:72:TRP:CZ3	2.49	0.48
1:A:66:THR:OG1	1:A:67:ARG:N	2.47	0.48
1:A:163:GLU:O	1:A:164:SER:C	2.56	0.48
1:C:158:ASN:O	1:C:159:LEU:CB	2.61	0.48
1:G:115:LEU:HD22	1:G:119:LEU:CD2	2.31	0.48
1:H:242:THR:O	1:H:242:THR:CG2	2.59	0.48
1:K:62:PRO:HG2	1:K:64:ASN:ND2	2.29	0.48
1:K:152:VAL:CG1	1:K:203:THR:HG22	2.43	0.48
1:S:247:LEU:HD12	1:S:288:PHE:CE1	2.49	0.48
1:T:80:ILE:N	1:T:81:PRO:HD2	2.29	0.48
1:F:231:TYR:O	1:F:234:VAL:N	2.46	0.47
1:H:343:PHE:CD1	1:H:343:PHE:C	2.92	0.47
1:J:261:ILE:C	1:J:263:ASN:H	2.20	0.47
1:N:286:SER:HB3	1:P:116:LYS:HZ3	1.78	0.47
1:P:251:LEU:HD13	1:P:255:LEU:HD22	1.95	0.47
1:Q:294:SER:O	1:Q:295:GLY:C	2.57	0.47
1:B:166:GLU:O	1:B:170:GLN:HG3	2.14	0.47
1:E:150:LEU:HG	1:E:175:LEU:HD11	1.96	0.47
1:F:294:SER:O	1:F:295:GLY:C	2.56	0.47
1:H:223:TYR:O	1:H:226:PRO:HD2	2.14	0.47
1:H:376:PHE:C	1:H:376:PHE:CD2	2.92	0.47
1:H:408:THR:O	1:H:409:ASP:CB	2.61	0.47
1:M:77:LYS:HD3	1:O:292:THR:HG22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:99:PHE:O	1:M:103:ASN:HB2	2.14	0.47
1:M:110:PRO:HG3	1:O:242:THR:HG21	1.95	0.47
1:N:299:VAL:HG11	1:N:301:HIS:CE1	2.49	0.47
1:T:194:PHE:CD1	1:T:207:ILE:HG12	2.49	0.47
1:T:208:LEU:O	1:T:209:SER:C	2.57	0.47
1:A:118:ILE:O	1:A:119:LEU:C	2.58	0.47
1:B:57:ILE:O	1:B:57:ILE:HG22	2.14	0.47
1:C:64:ASN:OD1	1:C:68:ARG:NH1	2.47	0.47
1:D:84:ILE:HG23	1:D:131:TRP:HB3	1.96	0.47
1:H:401:TYR:OH	1:H:412:ARG:HG3	2.14	0.47
1:I:348:ALA:O	1:I:349:LEU:HB2	2.13	0.47
1:J:66:THR:O	1:J:70:ILE:HD12	2.14	0.47
1:K:382:SER:O	1:K:383:THR:C	2.56	0.47
1:A:273:PHE:HE1	1:A:346:LEU:HD22	1.79	0.47
1:B:343:PHE:O	1:B:344:SER:C	2.56	0.47
1:D:283:ASP:OD1	1:D:284:PRO:N	2.48	0.47
1:G:25:LEU:O	1:G:26:THR:C	2.56	0.47
1:K:265:LEU:O	1:K:269:LEU:HB2	2.15	0.47
1:L:204:ARG:HB3	1:L:246:LEU:HD11	1.95	0.47
1:M:248:SER:O	1:M:252:SER:OG	2.33	0.47
1:O:3:LEU:O	1:O:3:LEU:HD23	2.13	0.47
1:O:14:LEU:HD13	1:O:57:ILE:HD13	1.96	0.47
1:P:35:TYR:C	1:P:35:TYR:HD1	2.20	0.47
1:P:261:ILE:O	1:P:263:ASN:N	2.47	0.47
1:P:297:TRP:O	1:P:298:GLU:CB	2.62	0.47
1:A:285:THR:HG21	1:I:173:GLU:HG2	1.97	0.47
1:B:10:LEU:O	1:B:11:TRP:C	2.57	0.47
1:C:74:ALA:O	1:C:78:THR:HG23	2.14	0.47
1:C:293:ALA:O	1:C:294:SER:HB3	2.15	0.47
1:E:90:VAL:HG11	1:E:139:CYS:HB3	1.96	0.47
1:F:230:PHE:O	1:F:234:VAL:HG23	2.14	0.47
1:I:6:LEU:HD23	1:I:6:LEU:C	2.38	0.47
1:I:140:ALA:O	1:I:141:GLU:C	2.56	0.47
1:N:72:TRP:O	1:N:76:LEU:HD22	2.14	0.47
1:N:410:LYS:C	1:N:412:ARG:H	2.22	0.47
1:B:380:LEU:HB2	1:D:184:ILE:HD11	1.96	0.47
1:F:269:LEU:HD22	1:F:273:PHE:CZ	2.49	0.47
1:J:221:ARG:HD2	1:J:224:GLU:OE2	2.14	0.47
1:S:366:SER:O	1:S:367:LYS:HB2	2.14	0.47
1:A:6:LEU:HD23	1:A:6:LEU:O	2.14	0.47
1:E:62:PRO:HG2	1:E:64:ASN:OD1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:35:TYR:C	1:G:35:TYR:HD1	2.21	0.47
1:H:156:ILE:O	1:H:157:GLU:C	2.57	0.47
1:I:262:CYS:HA	1:I:265:LEU:HB2	1.97	0.47
1:L:299:VAL:CG1	1:L:300:PHE:N	2.76	0.47
1:M:54:LEU:HD12	1:M:72:TRP:CZ3	2.49	0.47
1:M:96:GLN:O	1:M:100:PRO:HG2	2.14	0.47
1:M:210:VAL:O	1:M:214:VAL:HG23	2.14	0.47
1:M:217:ARG:O	1:M:219:GLY:N	2.47	0.47
1:M:234:VAL:HG21	1:M:253:PHE:CE1	2.49	0.47
1:N:194:PHE:CE1	1:N:207:ILE:HG12	2.50	0.47
1:O:96:GLN:O	1:O:97:ILE:HD13	2.15	0.47
1:S:148:VAL:HG21	1:S:193:CYS:CB	2.45	0.47
1:A:386:ASP:O	1:A:387:GLY:C	2.58	0.47
1:B:150:LEU:O	1:B:154:LYS:HB2	2.14	0.47
1:C:3:LEU:O	1:C:3:LEU:HD23	2.15	0.47
1:D:242:THR:HG22	1:D:243:SER:N	2.30	0.47
1:F:241:ASP:HA	1:F:299:VAL:HG13	1.97	0.47
1:F:341:GLN:O	1:F:345:ILE:HG22	2.15	0.47
1:H:261:ILE:O	1:H:263:ASN:N	2.47	0.47
1:Q:408:THR:O	1:Q:408:THR:HG23	2.15	0.47
1:R:151:TYR:HA	1:R:175:LEU:HD13	1.96	0.47
1:A:142:GLU:O	1:A:143:THR:C	2.57	0.47
1:C:185:GLN:HA	1:E:379:GLU:HG3	1.96	0.47
1:E:418:SER:OG	1:F:259:SER:HB2	2.15	0.47
1:G:238:ALA:HA	1:G:247:LEU:CD2	2.44	0.47
1:H:189:GLU:OE1	1:H:189:GLU:N	2.38	0.47
1:I:408:THR:O	1:I:409:ASP:HB2	2.15	0.47
1:J:401:TYR:CE2	1:J:412:ARG:HG3	2.50	0.47
1:M:51:ARG:HH22	1:M:92:GLU:CD	2.23	0.47
1:Q:405:THR:O	1:Q:409:ASP:HB3	2.15	0.47
1:A:247:LEU:O	1:A:250:ALA:HB3	2.14	0.47
1:A:343:PHE:C	1:A:343:PHE:CD1	2.92	0.47
1:A:366:SER:O	1:A:367:LYS:CB	2.62	0.47
1:C:90:VAL:CG2	1:C:142:GLU:HG2	2.45	0.47
1:D:80:ILE:CG2	1:D:81:PRO:HD3	2.45	0.47
1:E:144:ILE:O	1:E:148:VAL:HG23	2.15	0.47
1:H:71:LEU:O	1:H:75:VAL:HG23	2.15	0.47
1:K:191:SER:HB3	1:K:211:MSE:HE2	1.97	0.47
1:L:110:PRO:HG3	1:T:242:THR:CG2	2.45	0.47
1:M:366:SER:O	1:M:368:HIS:N	2.46	0.47
1:N:204:ARG:CZ	1:N:297:TRP:CZ2	2.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:297:TRP:O	1:Q:298:GLU:HB3	2.15	0.47
1:Q:420:ALA:HB2	1:R:420:ALA:HB2	1.96	0.47
1:B:79:VAL:C	1:B:81:PRO:HD2	2.40	0.46
1:N:58:TYR:HA	1:N:61:THR:O	2.14	0.46
1:N:80:ILE:HG23	1:N:81:PRO:HD3	1.97	0.46
1:Q:232:ASP:OD1	1:Q:271:ARG:NH2	2.48	0.46
1:B:99:PHE:C	1:B:99:PHE:HD1	2.24	0.46
1:J:231:TYR:CE2	1:J:235:LEU:HD11	2.50	0.46
1:L:220:PRO:HB2	1:L:221:ARG:HG3	1.97	0.46
1:L:250:ALA:O	1:L:254:ILE:HG23	2.15	0.46
1:O:50:ILE:O	1:O:54:LEU:HD22	2.16	0.46
1:Q:14:LEU:HD13	1:Q:57:ILE:HG21	1.96	0.46
1:Q:283:ASP:C	1:Q:283:ASP:OD1	2.58	0.46
1:B:151:TYR:HB2	1:B:175:LEU:HD13	1.97	0.46
1:D:350:TYR:O	1:D:351:PRO:C	2.56	0.46
1:G:204:ARG:NH2	1:G:297:TRP:CZ2	2.83	0.46
1:I:70:ILE:HG12	1:I:111:VAL:CG2	2.46	0.46
1:L:110:PRO:HG3	1:T:242:THR:HG21	1.98	0.46
1:L:209:SER:HA	1:L:249:TYR:CE1	2.50	0.46
1:M:76:LEU:HA	1:M:79:VAL:HG22	1.98	0.46
1:Q:47:SER:O	1:Q:48:GLN:C	2.58	0.46
1:T:104:SER:O	1:T:104:SER:OG	2.33	0.46
1:A:54:LEU:HD12	1:A:72:TRP:HZ3	1.80	0.46
1:A:130:GLU:OE1	1:A:136:ARG:NH1	2.48	0.46
1:E:187:PRO:O	1:E:191:SER:OG	2.34	0.46
1:H:176:VAL:O	1:H:177:ASN:C	2.59	0.46
1:H:235:LEU:O	1:H:239:GLU:HG3	2.15	0.46
1:J:251:LEU:HG	1:J:279:PHE:CE2	2.50	0.46
1:K:148:VAL:O	1:K:152:VAL:HG23	2.15	0.46
1:O:79:VAL:C	1:O:81:PRO:HD2	2.39	0.46
1:Q:35:TYR:C	1:Q:35:TYR:CD1	2.93	0.46
1:Q:140:ALA:O	1:Q:141:GLU:C	2.59	0.46
1:T:238:ALA:O	1:T:278:ARG:NH1	2.47	0.46
1:A:99:PHE:CD1	1:A:99:PHE:C	2.93	0.46
1:C:150:LEU:O	1:C:154:LYS:HB2	2.15	0.46
1:C:414:THR:O	1:C:415:ARG:C	2.58	0.46
1:D:101:PHE:O	1:D:105:PRO:HA	2.15	0.46
1:F:343:PHE:C	1:F:343:PHE:CD1	2.94	0.46
1:F:376:PHE:CD2	1:F:376:PHE:C	2.94	0.46
1:I:84:ILE:O	1:I:85:LEU:HD12	2.15	0.46
1:I:366:SER:O	1:I:367:LYS:CB	2.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:254:ILE:O	1:M:255:LEU:C	2.56	0.46
1:N:152:VAL:HG21	1:N:197:HIS:ND1	2.30	0.46
1:S:241:ASP:HA	1:S:299:VAL:CG1	2.46	0.46
1:A:110:PRO:HG3	1:C:242:THR:HG21	1.97	0.46
1:A:189:GLU:OE1	1:A:189:GLU:N	2.46	0.46
1:D:225:ILE:HB	1:D:226:PRO:HD3	1.97	0.46
1:J:230:PHE:O	1:J:234:VAL:HG23	2.16	0.46
1:L:5:SER:HA	1:L:8:LYS:HE2	1.98	0.46
1:M:364:TYR:O	1:M:366:SER:O	2.34	0.46
1:T:6:LEU:O	1:T:9:ALA:HB3	2.16	0.46
1:A:10:LEU:O	1:A:13:VAL:HG12	2.16	0.46
1:A:152:VAL:HG13	1:A:203:THR:HG22	1.96	0.46
1:F:131:TRP:O	1:F:135:LEU:HD12	2.16	0.46
1:H:270:TYR:HB3	1:H:370:PHE:CD2	2.50	0.46
1:K:149:ASP:OD1	1:K:197:HIS:NE2	2.49	0.46
1:L:396:SER:C	1:L:398:PHE:H	2.24	0.46
1:M:152:VAL:HG13	1:M:203:THR:HG22	1.98	0.46
1:N:47:SER:O	1:N:48:GLN:C	2.59	0.46
1:S:221:ARG:HB3	1:S:223:TYR:CZ	2.50	0.46
1:B:234:VAL:HG11	1:B:253:PHE:CD1	2.51	0.46
1:B:260:HIS:C	1:B:261:ILE:HG13	2.40	0.46
1:F:198:PHE:CD1	1:F:204:ARG:HG2	2.50	0.46
1:G:278:ARG:HD2	1:G:374:TYR:CZ	2.50	0.46
1:K:190:LEU:HD23	1:K:211:MSE:SE	2.65	0.46
1:N:215:ILE:O	1:N:216:ARG:C	2.58	0.46
1:O:32:VAL:O	1:O:33:GLU:C	2.59	0.46
1:P:184:ILE:HA	1:P:214:VAL:HG13	1.98	0.46
1:S:297:TRP:O	1:S:298:GLU:HB3	2.15	0.46
1:T:366:SER:O	1:T:367:LYS:CB	2.63	0.46
1:A:205:ILE:HB	1:A:206:PRO:HD3	1.98	0.46
1:B:73:LEU:O	1:B:74:ALA:C	2.59	0.46
1:E:140:ALA:O	1:E:144:ILE:HG22	2.16	0.46
1:G:189:GLU:OE1	1:G:189:GLU:N	2.49	0.46
1:H:300:PHE:CE1	1:H:301:HIS:O	2.69	0.46
1:J:243:SER:O	1:J:244:PRO:C	2.59	0.46
1:K:200:ASN:HA	1:K:201:PRO:HD3	1.82	0.46
1:M:221:ARG:HB3	1:M:223:TYR:CE2	2.51	0.46
1:O:348:ALA:O	1:O:349:LEU:HB2	2.15	0.46
1:R:217:ARG:HH11	1:R:217:ARG:HG2	1.81	0.46
1:A:77:LYS:HD3	1:C:292:THR:HG22	1.98	0.46
1:A:80:ILE:O	1:A:81:PRO:C	2.57	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:PHE:N	1:A:100:PRO:HD2	2.31	0.46
1:B:215:ILE:O	1:B:216:ARG:C	2.57	0.46
1:B:221:ARG:HB3	1:B:223:TYR:CE2	2.51	0.46
1:E:271:ARG:O	1:E:275:ILE:HG13	2.16	0.46
1:G:348:ALA:O	1:G:349:LEU:HB2	2.16	0.46
1:H:409:ASP:OD1	1:H:411:SER:OG	2.33	0.46
1:J:266:ASP:OD2	1:J:410:LYS:NZ	2.49	0.46
1:K:84:ILE:HG23	1:K:131:TRP:HB3	1.98	0.46
1:K:150:LEU:HG	1:K:175:LEU:HD11	1.99	0.46
1:K:204:ARG:CZ	1:K:297:TRP:CZ2	2.99	0.46
1:P:29:ILE:O	1:P:33:GLU:HG3	2.16	0.46
1:D:107:GLN:O	1:D:108:LEU:HD23	2.16	0.45
1:G:139:CYS:O	1:G:143:THR:OG1	2.32	0.45
1:I:1:MSE:HG2	1:I:4:GLN:OE1	2.16	0.45
1:I:363:LEU:O	1:I:363:LEU:HD23	2.16	0.45
1:I:414:THR:O	1:I:416:LEU:N	2.49	0.45
1:J:14:LEU:HD13	1:J:57:ILE:HG21	1.98	0.45
1:Q:348:ALA:O	1:Q:349:LEU:CB	2.64	0.45
1:T:429:ASN:C	1:T:431:VAL:H	2.24	0.45
1:B:363:LEU:CD2	1:B:367:LYS:HD3	2.46	0.45
1:D:80:ILE:HG22	1:D:81:PRO:HD3	1.98	0.45
1:E:185:GLN:HA	1:G:379:GLU:HG3	1.98	0.45
1:G:223:TYR:CD2	1:H:414:THR:HG21	2.51	0.45
1:H:353:ASN:OD1	1:H:407:LEU:HD11	2.17	0.45
1:J:268:SER:O	1:J:271:ARG:N	2.49	0.45
1:K:297:TRP:O	1:K:298:GLU:CB	2.64	0.45
1:L:181:HIS:O	1:L:185:GLN:HG3	2.16	0.45
1:O:215:ILE:HG22	1:O:256:MSE:HB3	1.99	0.45
1:Q:94:TRP:CD1	1:Q:146:ARG:NE	2.84	0.45
1:E:132:GLY:O	1:E:135:LEU:HD12	2.17	0.45
1:E:137:ARG:HB2	1:E:137:ARG:CZ	2.46	0.45
1:E:223:TYR:CD2	1:F:414:THR:HG21	2.51	0.45
1:G:220:PRO:HB2	1:G:221:ARG:HG3	1.98	0.45
1:H:297:TRP:O	1:H:298:GLU:CB	2.65	0.45
1:H:408:THR:O	1:H:409:ASP:HB2	2.15	0.45
1:I:42:GLN:NE2	1:I:131:TRP:HE1	2.13	0.45
1:L:231:TYR:CZ	1:L:235:LEU:HD11	2.51	0.45
1:Q:1:MSE:HG2	1:Q:4:GLN:HB2	1.98	0.45
1:Q:201:PRO:HB3	1:Q:300:PHE:HB2	1.98	0.45
1:A:176:VAL:O	1:A:180:VAL:HG23	2.17	0.45
1:A:199:LEU:O	1:A:201:PRO:HD3	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:LEU:HD11	1:B:154:LYS:HE3	1.98	0.45
1:E:67:ARG:O	1:E:71:LEU:HB2	2.17	0.45
1:E:109:LYS:N	1:E:110:PRO:CD	2.80	0.45
1:G:107:GLN:NE2	1:G:170:GLN:HE22	2.15	0.45
1:H:25:LEU:O	1:H:26:THR:C	2.58	0.45
1:L:244:PRO:O	1:L:245:ILE:C	2.59	0.45
1:L:351:PRO:HG3	1:L:395:HIS:CE1	2.52	0.45
1:O:268:SER:O	1:O:272:LEU:HG	2.16	0.45
1:R:139:CYS:O	1:R:140:ALA:C	2.60	0.45
1:R:401:TYR:CZ	1:R:412:ARG:CG	2.92	0.45
1:S:65:ASN:OD1	1:S:67:ARG:N	2.50	0.45
1:T:401:TYR:OH	1:T:412:ARG:HG3	2.17	0.45
1:C:358:LEU:O	1:C:359:ARG:HB3	2.15	0.45
1:H:354:PHE:CE1	1:H:358:LEU:HD11	2.52	0.45
1:H:414:THR:C	1:H:416:LEU:H	2.25	0.45
1:I:278:ARG:HD2	1:I:374:TYR:CE1	2.52	0.45
1:I:283:ASP:HA	1:I:284:PRO:HD3	1.75	0.45
1:K:101:PHE:CD1	1:K:101:PHE:C	2.94	0.45
1:N:201:PRO:HB2	1:N:202:PRO:HD3	1.99	0.45
1:O:352:ILE:HG12	1:O:398:PHE:CE1	2.51	0.45
1:P:99:PHE:C	1:P:99:PHE:CD1	2.94	0.45
1:P:351:PRO:HG3	1:P:395:HIS:ND1	2.32	0.45
1:Q:261:ILE:HG21	1:Q:264:SER:HB2	1.99	0.45
1:T:266:ASP:N	1:T:266:ASP:OD1	2.49	0.45
1:C:275:ILE:O	1:C:276:TYR:C	2.60	0.45
1:E:14:LEU:HD13	1:E:57:ILE:HG21	1.97	0.45
1:L:281:MSE:HE1	1:L:380:LEU:HG	1.96	0.45
1:N:109:LYS:N	1:N:110:PRO:CD	2.80	0.45
1:N:204:ARG:O	1:N:205:ILE:C	2.60	0.45
1:A:350:TYR:N	1:A:351:PRO:CD	2.79	0.45
1:B:80:ILE:N	1:B:81:PRO:CD	2.80	0.45
1:C:245:ILE:O	1:C:249:TYR:HD2	2.00	0.45
1:D:6:LEU:HD23	1:D:10:LEU:HD13	1.99	0.45
1:D:99:PHE:HB3	1:D:100:PRO:HD3	1.99	0.45
1:G:389:LEU:C	1:G:391:ARG:H	2.25	0.45
1:I:404:GLU:O	1:I:407:LEU:N	2.50	0.45
1:J:204:ARG:CZ	1:J:297:TRP:CZ2	3.00	0.45
1:J:342:LEU:HA	1:J:345:ILE:HG22	1.99	0.45
1:N:99:PHE:HB3	1:N:100:PRO:HD3	1.97	0.45
1:N:366:SER:O	1:N:367:LYS:CB	2.65	0.45
1:P:32:VAL:HG13	1:P:82:LEU:HD21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:141:GLU:O	1:Q:145:THR:OG1	2.29	0.45
1:B:80:ILE:N	1:B:81:PRO:HD2	2.32	0.45
1:B:99:PHE:HB3	1:B:100:PRO:HD3	1.99	0.45
1:C:102:LEU:HD13	1:C:175:LEU:HD21	1.99	0.45
1:F:268:SER:O	1:F:271:ARG:N	2.49	0.45
1:H:176:VAL:HG12	1:H:180:VAL:HG23	1.98	0.45
1:I:251:LEU:HD22	1:I:255:LEU:HD22	1.98	0.45
1:I:268:SER:O	1:I:269:LEU:C	2.59	0.45
1:I:347:TYR:O	1:I:351:PRO:HB3	2.17	0.45
1:N:238:ALA:O	1:N:278:ARG:NH1	2.49	0.45
1:Q:343:PHE:C	1:Q:343:PHE:CD1	2.94	0.45
1:B:242:THR:HB	1:B:301:HIS:HA	1.97	0.45
1:C:410:LYS:C	1:C:412:ARG:H	2.25	0.45
1:D:61:THR:O	1:D:61:THR:OG1	2.31	0.45
1:E:80:ILE:N	1:E:81:PRO:HD2	2.32	0.45
1:H:11:TRP:O	1:H:15:HIS:ND1	2.47	0.45
1:I:176:VAL:O	1:I:180:VAL:HG23	2.16	0.45
1:K:151:TYR:HA	1:K:175:LEU:CD1	2.47	0.45
1:K:151:TYR:CA	1:K:175:LEU:HD13	2.46	0.45
1:L:247:LEU:CD1	1:L:288:PHE:CD1	3.00	0.45
1:L:345:ILE:O	1:L:345:ILE:CG1	2.65	0.45
1:R:247:LEU:HD12	1:R:288:PHE:CD1	2.52	0.45
1:S:213:GLU:OE1	1:S:216:ARG:HD2	2.17	0.45
1:A:97:ILE:CA	1:A:100:PRO:HG2	2.47	0.45
1:A:242:THR:HB	1:A:301:HIS:HA	1.99	0.45
1:B:261:ILE:HG21	1:B:264:SER:HB2	1.99	0.45
1:J:84:ILE:HG23	1:J:131:TRP:HB3	1.99	0.45
1:Q:99:PHE:CZ	1:Q:103:ASN:OD1	2.70	0.45
1:T:76:LEU:HG	1:T:93:TRP:CZ3	2.52	0.45
1:A:164:SER:O	1:A:165:GLN:C	2.60	0.44
1:A:205:ILE:O	1:A:209:SER:HB2	2.16	0.44
1:A:283:ASP:CG	1:A:284:PRO:HD2	2.42	0.44
1:A:293:ALA:O	1:A:294:SER:CB	2.65	0.44
1:E:269:LEU:HD22	1:E:273:PHE:CE1	2.51	0.44
1:F:6:LEU:HD23	1:F:6:LEU:C	2.42	0.44
1:H:101:PHE:CD1	1:H:101:PHE:C	2.95	0.44
1:H:129:ASP:O	1:H:130:GLU:C	2.60	0.44
1:L:184:ILE:HD11	1:T:380:LEU:HB2	1.98	0.44
1:L:348:ALA:O	1:L:349:LEU:CB	2.64	0.44
1:N:145:THR:O	1:N:146:ARG:C	2.59	0.44
1:N:176:VAL:HG12	1:N:177:ASN:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:10:LEU:HD13	1:O:28:LEU:HD13	1.99	0.44
1:P:292:THR:OG1	1:P:293:ALA:N	2.50	0.44
1:Q:266:ASP:N	1:Q:266:ASP:OD1	2.50	0.44
1:S:86:ASP:O	1:S:87:ARG:C	2.59	0.44
1:B:223:TYR:O	1:B:226:PRO:HD2	2.17	0.44
1:D:217:ARG:O	1:D:218:GLN:C	2.59	0.44
1:E:401:TYR:CE1	1:E:412:ARG:HG3	2.52	0.44
1:F:251:LEU:HD22	1:F:255:LEU:HD22	1.99	0.44
1:K:172:ILE:HG13	1:K:173:GLU:N	2.31	0.44
1:N:401:TYR:CE2	1:N:412:ARG:HG3	2.53	0.44
1:O:363:LEU:CD2	1:O:367:LYS:HD2	2.47	0.44
1:O:377:ASN:HB3	1:O:380:LEU:HB3	1.98	0.44
1:P:46:ASN:O	1:P:47:SER:C	2.60	0.44
1:P:422:VAL:O	1:P:426:ASN:ND2	2.50	0.44
1:A:261:ILE:O	1:A:263:ASN:N	2.50	0.44
1:A:278:ARG:HD2	1:A:374:TYR:CZ	2.51	0.44
1:B:185:GLN:HA	1:J:379:GLU:HG3	1.99	0.44
1:E:243:SER:HB3	1:E:246:LEU:HB3	1.99	0.44
1:G:63:PHE:CE1	1:G:69:ARG:HG2	2.53	0.44
1:M:108:LEU:HB2	1:M:111:VAL:HG23	1.98	0.44
1:M:389:LEU:C	1:M:391:ARG:H	2.26	0.44
1:Q:204:ARG:NH2	1:Q:297:TRP:CZ2	2.85	0.44
1:S:140:ALA:O	1:S:144:ILE:HG22	2.16	0.44
1:T:261:ILE:HG21	1:T:264:SER:HB2	1.99	0.44
1:C:27:GLU:O	1:C:30:ALA:HB3	2.18	0.44
1:C:255:LEU:HD12	1:C:255:LEU:HA	1.84	0.44
1:D:86:ASP:O	1:D:87:ARG:C	2.60	0.44
1:G:276:TYR:HE2	1:G:358:LEU:HD21	1.82	0.44
1:G:297:TRP:O	1:G:298:GLU:CB	2.64	0.44
1:H:51:ARG:NH2	1:H:92:GLU:OE2	2.50	0.44
1:I:47:SER:O	1:I:49:LYS:N	2.50	0.44
1:L:80:ILE:N	1:L:81:PRO:HD2	2.32	0.44
1:M:102:LEU:O	1:M:171:THR:HG23	2.17	0.44
1:M:251:LEU:O	1:M:252:SER:C	2.59	0.44
1:P:215:ILE:CD1	1:P:222:LEU:HD22	2.46	0.44
1:Q:99:PHE:HB3	1:Q:100:PRO:CD	2.47	0.44
1:S:251:LEU:HD22	1:S:255:LEU:HD13	1.99	0.44
1:S:343:PHE:CD1	1:S:343:PHE:C	2.95	0.44
1:A:357:PHE:CE1	1:A:361:PRO:HB3	2.52	0.44
1:B:360:ASP:CG	1:B:363:LEU:HB2	2.43	0.44
1:D:379:GLU:HG3	1:F:185:GLN:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:152:VAL:HG12	1:E:156:ILE:HD11	2.00	0.44
1:F:99:PHE:HB3	1:F:100:PRO:CD	2.48	0.44
1:L:35:TYR:C	1:L:35:TYR:CD1	2.95	0.44
1:L:109:LYS:N	1:L:110:PRO:CD	2.81	0.44
1:M:217:ARG:HD3	1:M:217:ARG:HA	1.77	0.44
1:N:251:LEU:O	1:N:254:ILE:N	2.51	0.44
1:O:251:LEU:HD13	1:O:255:LEU:CD2	2.47	0.44
1:O:293:ALA:O	1:O:294:SER:CB	2.65	0.44
1:Q:366:SER:O	1:Q:367:LYS:CB	2.66	0.44
1:S:205:ILE:CB	1:S:206:PRO:CD	2.95	0.44
1:T:171:THR:HG22	1:T:175:LEU:HD12	1.99	0.44
1:A:1:MSE:O	1:A:1:MSE:HG2	2.17	0.44
1:A:247:LEU:HD13	1:A:288:PHE:CE2	2.53	0.44
1:B:230:PHE:O	1:B:231:TYR:C	2.60	0.44
1:B:363:LEU:HD23	1:B:363:LEU:C	2.43	0.44
1:B:383:THR:HG22	1:B:384:LYS:N	2.32	0.44
1:D:241:ASP:O	1:D:247:LEU:HD11	2.18	0.44
1:G:117:SER:OG	1:I:375:SER:HB2	2.18	0.44
1:J:203:THR:O	1:J:206:PRO:HD2	2.17	0.44
1:K:25:LEU:N	1:K:25:LEU:HD12	2.33	0.44
1:O:200:ASN:OD1	1:O:202:PRO:HD2	2.18	0.44
1:R:154:LYS:O	1:R:168:ARG:HD2	2.17	0.44
1:S:76:LEU:O	1:S:80:ILE:HG22	2.18	0.44
1:T:3:LEU:HD12	1:T:46:ASN:ND2	2.32	0.44
1:T:181:HIS:O	1:T:185:GLN:HG3	2.18	0.44
1:T:261:ILE:CG2	1:T:264:SER:HB2	2.48	0.44
1:A:87:ARG:NH1	1:A:142:GLU:OE1	2.51	0.44
1:A:209:SER:HA	1:A:249:TYR:CE1	2.53	0.44
1:D:70:ILE:HG12	1:D:111:VAL:CG2	2.47	0.44
1:D:99:PHE:O	1:D:100:PRO:C	2.60	0.44
1:E:102:LEU:O	1:E:171:THR:HG23	2.18	0.44
1:F:80:ILE:N	1:F:81:PRO:CD	2.81	0.44
1:J:234:VAL:O	1:J:237:CYS:HB3	2.18	0.44
1:L:404:GLU:CD	1:L:404:GLU:H	2.25	0.44
1:P:158:ASN:O	1:P:159:LEU:CB	2.66	0.44
1:S:3:LEU:HD23	1:S:7:VAL:CG2	2.48	0.44
1:E:110:PRO:O	1:E:114:ASP:OD1	2.36	0.44
1:E:198:PHE:CE1	1:E:204:ARG:HG2	2.53	0.44
1:I:205:ILE:O	1:I:206:PRO:C	2.61	0.44
1:J:32:VAL:CG1	1:J:82:LEU:HD21	2.40	0.44
1:K:368:HIS:O	1:K:369:ASN:CB	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:402:THR:HG22	1:T:359:ARG:NH1	2.33	0.44
1:P:386:ASP:HB2	1:Q:399:LEU:HD12	1.98	0.44
1:B:26:THR:HG23	1:J:295:GLY:O	2.18	0.44
1:C:215:ILE:O	1:C:216:ARG:C	2.59	0.44
1:C:420:ALA:HB2	1:D:420:ALA:HB2	2.00	0.44
1:J:113:SER:O	1:J:116:LYS:HB2	2.18	0.44
1:N:14:LEU:CD1	1:N:57:ILE:HG21	2.48	0.44
1:O:208:LEU:HD21	1:O:234:VAL:HG22	2.00	0.44
1:R:3:LEU:O	1:R:3:LEU:HD22	2.18	0.44
1:R:237:CYS:HA	1:R:241:ASP:OD2	2.18	0.44
1:S:280:SER:O	1:S:281:MSE:HE2	2.18	0.44
1:T:115:LEU:HD22	1:T:119:LEU:CD2	2.48	0.44
1:T:129:ASP:O	1:T:130:GLU:C	2.59	0.44
1:A:355:LEU:HD13	1:J:398:PHE:HB3	2.00	0.43
1:B:65:ASN:HD21	1:B:68:ARG:HG3	1.83	0.43
1:B:222:LEU:O	1:B:223:TYR:C	2.58	0.43
1:F:64:ASN:OD1	1:F:68:ARG:NH1	2.50	0.43
1:M:64:ASN:OD1	1:M:64:ASN:N	2.51	0.43
1:M:101:PHE:CD1	1:M:115:LEU:HD12	2.53	0.43
1:N:278:ARG:HD2	1:N:374:TYR:CZ	2.52	0.43
1:O:243:SER:O	1:O:244:PRO:C	2.60	0.43
1:R:408:THR:O	1:R:408:THR:HG23	2.17	0.43
1:T:35:TYR:C	1:T:35:TYR:CD1	2.95	0.43
1:B:25:LEU:O	1:B:28:LEU:N	2.51	0.43
1:B:377:ASN:C	1:B:377:ASN:OD1	2.60	0.43
1:B:379:GLU:H	1:B:379:GLU:HG2	1.63	0.43
1:G:32:VAL:HG13	1:G:82:LEU:CD2	2.45	0.43
1:H:10:LEU:O	1:H:14:LEU:HD12	2.18	0.43
1:H:239:GLU:O	1:H:374:TYR:OH	2.33	0.43
1:H:242:THR:HG21	1:J:110:PRO:CG	2.48	0.43
1:H:350:TYR:N	1:H:351:PRO:CD	2.81	0.43
1:K:297:TRP:O	1:K:298:GLU:HB3	2.18	0.43
1:P:115:LEU:HD22	1:P:119:LEU:HD22	1.99	0.43
1:P:205:ILE:HB	1:P:206:PRO:HD3	1.99	0.43
1:Q:293:ALA:C	1:Q:295:GLY:N	2.74	0.43
1:R:267:ASP:N	1:R:267:ASP:OD1	2.51	0.43
1:R:273:PHE:HB3	1:R:357:PHE:CZ	2.53	0.43
1:R:297:TRP:O	1:R:298:GLU:CB	2.67	0.43
1:A:185:GLN:HG2	1:C:379:GLU:HG2	2.01	0.43
1:A:204:ARG:CZ	1:A:297:TRP:CZ2	3.01	0.43
1:A:285:THR:HG23	1:I:173:GLU:OE2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:151:TYR:HA	1:D:175:LEU:HD13	2.00	0.43
1:D:242:THR:O	1:D:247:LEU:HD12	2.17	0.43
1:D:248:SER:O	1:D:252:SER:OG	2.36	0.43
1:E:194:PHE:CG	1:E:207:ILE:HG23	2.54	0.43
1:F:386:ASP:C	1:F:388:LEU:N	2.75	0.43
1:G:10:LEU:O	1:G:14:LEU:HD12	2.18	0.43
1:G:354:PHE:O	1:G:357:PHE:HB3	2.18	0.43
1:H:172:ILE:O	1:H:176:VAL:HG23	2.19	0.43
1:I:62:PRO:HG2	1:I:64:ASN:ND2	2.34	0.43
1:M:238:ALA:O	1:M:278:ARG:NH1	2.50	0.43
1:M:269:LEU:HD21	1:M:273:PHE:CE1	2.52	0.43
1:N:189:GLU:O	1:N:192:SER:N	2.45	0.43
1:O:177:ASN:C	1:O:177:ASN:OD1	2.61	0.43
1:P:414:THR:O	1:P:415:ARG:C	2.61	0.43
1:R:280:SER:C	1:R:281:MSE:HE2	2.43	0.43
1:S:221:ARG:HB3	1:S:223:TYR:CE2	2.54	0.43
1:D:25:LEU:N	1:D:25:LEU:HD12	2.33	0.43
1:D:115:LEU:HD22	1:D:119:LEU:HD22	2.00	0.43
1:E:83:LEU:N	1:E:83:LEU:HD23	2.32	0.43
1:H:430:ALA:O	1:H:431:VAL:HB	2.19	0.43
1:J:151:TYR:CA	1:J:175:LEU:HD13	2.48	0.43
1:K:266:ASP:OD1	1:K:266:ASP:N	2.51	0.43
1:K:270:TYR:O	1:K:271:ARG:C	2.61	0.43
1:M:63:PHE:CE2	1:M:69:ARG:HG2	2.53	0.43
1:N:46:ASN:HA	1:N:49:LYS:HB2	2.00	0.43
1:N:217:ARG:HG2	1:N:217:ARG:NH1	2.33	0.43
1:O:99:PHE:C	1:O:99:PHE:HD1	2.26	0.43
1:Q:415:ARG:O	1:Q:419:ILE:HG23	2.18	0.43
1:R:119:LEU:O	1:R:123:LEU:HD22	2.18	0.43
1:R:127:ASP:HB3	1:R:130:GLU:HB2	2.00	0.43
1:R:396:SER:HB3	1:S:386:ASP:OD1	2.18	0.43
1:S:350:TYR:N	1:S:351:PRO:CD	2.81	0.43
1:B:101:PHE:CD1	1:B:115:LEU:HD12	2.53	0.43
1:B:378:GLN:O	1:B:381:LEU:HB3	2.17	0.43
1:F:268:SER:O	1:F:269:LEU:C	2.61	0.43
1:J:246:LEU:O	1:J:249:TYR:HB2	2.19	0.43
1:O:49:LYS:O	1:O:52:HIS:HB2	2.18	0.43
1:S:352:ILE:HG13	1:S:406:GLU:OE2	2.18	0.43
1:B:3:LEU:HD12	1:B:46:ASN:ND2	2.33	0.43
1:D:382:SER:O	1:D:383:THR:C	2.60	0.43
1:I:11:TRP:O	1:I:12:ASN:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:137:ARG:HB2	1:M:137:ARG:CZ	2.49	0.43
1:M:223:TYR:CD2	1:N:414:THR:HG21	2.54	0.43
1:M:410:LYS:C	1:M:412:ARG:N	2.76	0.43
1:O:35:TYR:CE1	1:O:39:TYR:HB2	2.53	0.43
1:P:221:ARG:HB3	1:P:223:TYR:CE2	2.54	0.43
1:S:130:GLU:OE1	1:S:136:ARG:NH1	2.52	0.43
1:D:241:ASP:HA	1:D:299:VAL:HG13	2.01	0.43
1:D:286:SER:HB3	1:F:116:LYS:HZ2	1.83	0.43
1:D:430:ALA:O	1:D:431:VAL:HB	2.18	0.43
1:E:53:ILE:O	1:E:57:ILE:HG13	2.18	0.43
1:F:43:ASN:HA	1:F:44:PRO:HD2	1.85	0.43
1:F:185:GLN:O	1:F:221:ARG:NH2	2.52	0.43
1:G:107:GLN:OE1	1:G:170:GLN:NE2	2.51	0.43
1:H:210:VAL:O	1:H:214:VAL:HG23	2.19	0.43
1:H:266:ASP:OD1	1:H:266:ASP:N	2.51	0.43
1:H:422:VAL:O	1:H:426:ASN:ND2	2.52	0.43
1:J:238:ALA:O	1:J:278:ARG:NH1	2.51	0.43
1:L:84:ILE:C	1:L:85:LEU:HD12	2.44	0.43
1:M:269:LEU:CD2	1:M:273:PHE:CE1	3.02	0.43
1:P:379:GLU:H	1:P:379:GLU:HG2	1.67	0.43
1:R:247:LEU:HD23	1:R:247:LEU:HA	1.87	0.43
1:R:293:ALA:O	1:R:295:GLY:N	2.52	0.43
1:T:86:ASP:O	1:T:87:ARG:C	2.61	0.43
1:D:250:ALA:O	1:D:251:LEU:C	2.61	0.43
1:E:343:PHE:O	1:E:344:SER:C	2.62	0.43
1:G:46:ASN:O	1:G:50:ILE:HG13	2.19	0.43
1:G:268:SER:O	1:G:269:LEU:C	2.60	0.43
1:H:86:ASP:O	1:H:89:ALA:HB3	2.19	0.43
1:H:244:PRO:O	1:H:245:ILE:C	2.62	0.43
1:J:101:PHE:CD1	1:J:101:PHE:C	2.96	0.43
1:J:209:SER:HA	1:J:249:TYR:CE1	2.54	0.43
1:K:73:LEU:HD12	1:K:111:VAL:HG13	2.01	0.43
1:M:259:SER:OG	1:M:260:HIS:CD2	2.71	0.43
1:O:79:VAL:O	1:O:82:LEU:HB2	2.19	0.43
1:O:155:ALA:O	1:O:156:ILE:HG13	2.19	0.43
1:P:234:VAL:O	1:P:237:CYS:HB3	2.18	0.43
1:Q:277:LEU:HD23	1:Q:277:LEU:O	2.18	0.43
1:S:408:THR:O	1:S:408:THR:CG2	2.64	0.43
1:D:271:ARG:HH11	1:D:271:ARG:HG3	1.84	0.43
1:I:194:PHE:CD1	1:I:207:ILE:HG12	2.53	0.43
1:L:270:TYR:OH	1:L:368:HIS:HD2	2.02	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:198:PHE:CE1	1:O:204:ARG:HG2	2.54	0.43
1:P:99:PHE:N	1:P:100:PRO:HD2	2.34	0.43
1:R:348:ALA:O	1:R:349:LEU:HB2	2.18	0.43
1:S:150:LEU:HG	1:S:175:LEU:HD11	2.00	0.43
1:A:185:GLN:O	1:A:186:ARG:HD3	2.18	0.43
1:C:217:ARG:HG2	1:C:217:ARG:NH1	2.34	0.43
1:G:364:TYR:CE1	1:G:368:HIS:CD2	3.07	0.43
1:H:272:LEU:O	1:H:273:PHE:C	2.61	0.43
1:H:281:MSE:O	1:H:282:ILE:C	2.62	0.43
1:J:107:GLN:O	1:J:108:LEU:HD23	2.19	0.43
1:K:243:SER:O	1:K:244:PRO:C	2.62	0.43
1:N:282:ILE:HD12	1:N:288:PHE:CZ	2.54	0.43
1:T:94:TRP:CH2	1:T:146:ARG:HB3	2.54	0.43
1:C:242:THR:HB	1:C:301:HIS:HA	2.01	0.42
1:F:130:GLU:OE1	1:F:136:ARG:NH1	2.52	0.42
1:F:417:ASP:O	1:F:421:VAL:HG23	2.19	0.42
1:G:72:TRP:O	1:G:76:LEU:HB2	2.19	0.42
1:H:81:PRO:HA	1:H:121:TYR:OH	2.19	0.42
1:H:230:PHE:O	1:H:234:VAL:HG23	2.18	0.42
1:H:243:SER:O	1:H:244:PRO:C	2.58	0.42
1:I:125:PHE:CD2	1:I:125:PHE:N	2.87	0.42
1:K:172:ILE:O	1:K:173:GLU:C	2.62	0.42
1:K:247:LEU:HD12	1:K:288:PHE:CD1	2.54	0.42
1:K:271:ARG:H	1:K:271:ARG:HG2	1.62	0.42
1:N:208:LEU:HD23	1:N:208:LEU:HA	1.86	0.42
1:O:94:TRP:HA	1:O:98:PHE:CD2	2.54	0.42
1:P:48:GLN:O	1:P:52:HIS:HB2	2.18	0.42
1:Q:69:ARG:O	1:Q:70:ILE:C	2.62	0.42
1:Q:221:ARG:HB3	1:Q:223:TYR:CE2	2.54	0.42
1:Q:297:TRP:O	1:Q:298:GLU:CB	2.65	0.42
1:R:47:SER:O	1:R:51:ARG:HG3	2.19	0.42
1:A:142:GLU:O	1:A:145:THR:N	2.52	0.42
1:A:270:TYR:O	1:A:271:ARG:C	2.60	0.42
1:B:235:LEU:O	1:B:236:LYS:C	2.60	0.42
1:D:150:LEU:HG	1:D:175:LEU:HD11	2.00	0.42
1:I:386:ASP:O	1:I:387:GLY:C	2.62	0.42
1:K:109:LYS:N	1:K:110:PRO:CD	2.82	0.42
1:L:194:PHE:CD1	1:L:207:ILE:HG12	2.54	0.42
1:M:86:ASP:H	1:M:89:ALA:HB3	1.83	0.42
1:P:3:LEU:O	1:P:7:VAL:HG23	2.19	0.42
1:T:153:SER:OG	1:T:154:LYS:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:430:ALA:O	1:B:431:VAL:CB	2.67	0.42
1:C:299:VAL:HG12	1:C:300:PHE:N	2.33	0.42
1:F:366:SER:O	1:F:367:LYS:CB	2.65	0.42
1:G:366:SER:O	1:G:367:LYS:HB2	2.18	0.42
1:H:63:PHE:CE2	1:H:69:ARG:HG2	2.54	0.42
1:H:251:LEU:O	1:H:252:SER:C	2.62	0.42
1:H:261:ILE:HG22	1:H:262:CYS:N	2.34	0.42
1:H:378:GLN:O	1:H:379:GLU:C	2.62	0.42
1:J:50:ILE:O	1:J:54:LEU:HD22	2.19	0.42
1:J:136:ARG:HD2	1:J:136:ARG:HA	1.66	0.42
1:L:47:SER:O	1:L:51:ARG:HG3	2.20	0.42
1:M:125:PHE:C	1:M:125:PHE:CD1	2.97	0.42
1:M:217:ARG:HG2	1:M:217:ARG:HH11	1.84	0.42
1:O:241:ASP:O	1:O:278:ARG:NH2	2.37	0.42
1:P:152:VAL:HG11	1:P:197:HIS:ND1	2.35	0.42
1:R:189:GLU:OE1	1:R:189:GLU:N	2.50	0.42
1:S:296:ASN:OD1	1:S:296:ASN:N	2.52	0.42
1:T:276:TYR:HB2	1:T:342:LEU:HD23	2.01	0.42
1:D:251:LEU:HD23	1:D:251:LEU:HA	1.87	0.42
1:F:376:PHE:CD2	1:F:376:PHE:O	2.73	0.42
1:H:65:ASN:OD1	1:H:65:ASN:C	2.62	0.42
1:M:62:PRO:CG	1:M:64:ASN:ND2	2.81	0.42
1:O:115:LEU:HD22	1:O:119:LEU:HD22	2.00	0.42
1:P:261:ILE:HG22	1:P:262:CYS:N	2.34	0.42
1:Q:389:LEU:O	1:Q:392:HIS:N	2.51	0.42
1:R:424:LEU:HD23	1:R:424:LEU:O	2.19	0.42
1:B:101:PHE:CD1	1:B:101:PHE:C	2.97	0.42
1:B:299:VAL:HG12	1:B:300:PHE:N	2.33	0.42
1:C:65:ASN:OD1	1:C:65:ASN:C	2.62	0.42
1:D:13:VAL:O	1:D:13:VAL:HG13	2.18	0.42
1:F:3:LEU:HD23	1:F:3:LEU:O	2.19	0.42
1:G:86:ASP:HB3	1:G:135:LEU:HD21	2.01	0.42
1:H:282:ILE:HD12	1:H:288:PHE:CZ	2.54	0.42
1:H:414:THR:C	1:H:416:LEU:N	2.77	0.42
1:I:230:PHE:O	1:I:234:VAL:HG23	2.18	0.42
1:I:279:PHE:CD2	1:I:288:PHE:HE2	2.37	0.42
1:J:152:VAL:CG1	1:J:203:THR:HG22	2.45	0.42
1:J:343:PHE:O	1:J:344:SER:C	2.63	0.42
1:L:191:SER:HB3	1:L:211:MSE:HE2	2.01	0.42
1:P:80:ILE:N	1:P:81:PRO:HD2	2.34	0.42
1:Q:208:LEU:O	1:Q:209:SER:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:220:PRO:HA	1:Q:221:ARG:HA	1.82	0.42
1:R:253:PHE:CD1	1:R:253:PHE:C	2.98	0.42
1:S:99:PHE:CD1	1:S:99:PHE:C	2.98	0.42
1:F:98:PHE:CD1	1:F:115:LEU:HD21	2.54	0.42
1:H:188:LYS:O	1:H:191:SER:OG	2.28	0.42
1:H:217:ARG:HD3	1:H:217:ARG:HA	1.93	0.42
1:H:424:LEU:HD22	1:H:428:LEU:CD2	2.50	0.42
1:K:80:ILE:N	1:K:81:PRO:CD	2.82	0.42
1:K:99:PHE:O	1:K:100:PRO:C	2.63	0.42
1:M:424:LEU:HD22	1:M:428:LEU:CD2	2.49	0.42
1:N:6:LEU:O	1:N:9:ALA:N	2.52	0.42
1:O:430:ALA:O	1:O:431:VAL:CB	2.66	0.42
1:P:348:ALA:O	1:P:349:LEU:HB2	2.19	0.42
1:R:91:GLY:O	1:R:92:GLU:C	2.62	0.42
1:T:372:ILE:HA	1:T:372:ILE:HD13	1.72	0.42
1:A:79:VAL:C	1:A:81:PRO:HD2	2.44	0.42
1:A:233:LEU:O	1:A:236:LYS:N	2.53	0.42
1:A:396:SER:C	1:A:398:PHE:N	2.78	0.42
1:B:109:LYS:N	1:B:110:PRO:CD	2.82	0.42
1:C:32:VAL:HG13	1:C:82:LEU:HD21	2.02	0.42
1:C:62:PRO:HG2	1:C:64:ASN:ND2	2.35	0.42
1:D:116:LYS:O	1:D:117:SER:C	2.62	0.42
1:H:62:PRO:HG2	1:H:64:ASN:HD21	1.84	0.42
1:H:218:GLN:OE1	1:H:260:HIS:NE2	2.42	0.42
1:I:293:ALA:O	1:I:294:SER:HB3	2.19	0.42
1:J:351:PRO:HG2	1:J:406:GLU:OE2	2.19	0.42
1:O:208:LEU:O	1:O:212:VAL:HG13	2.20	0.42
1:P:49:LYS:O	1:P:53:ILE:HG12	2.19	0.42
1:R:262:CYS:HA	1:R:265:LEU:HD12	2.01	0.42
1:S:121:TYR:CD2	1:S:121:TYR:C	2.97	0.42
1:T:99:PHE:CD1	1:T:99:PHE:C	2.97	0.42
1:D:366:SER:O	1:D:367:LYS:CB	2.67	0.42
1:E:134:ASP:O	1:E:136:ARG:N	2.53	0.42
1:F:42:GLN:HB3	1:F:84:ILE:HD11	2.00	0.42
1:G:176:VAL:O	1:G:180:VAL:HG23	2.20	0.42
1:K:110:PRO:HG3	1:M:242:THR:CG2	2.50	0.42
1:L:150:LEU:HG	1:L:175:LEU:HD11	2.02	0.42
1:M:34:SER:O	1:M:35:TYR:C	2.62	0.42
1:M:404:GLU:O	1:M:408:THR:HG22	2.18	0.42
1:N:187:PRO:O	1:N:191:SER:OG	2.38	0.42
1:N:293:ALA:O	1:N:294:SER:CB	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:65:ASN:O	1:O:69:ARG:HG3	2.19	0.42
1:Q:14:LEU:CD1	1:Q:57:ILE:HG21	2.49	0.42
1:Q:273:PHE:HB3	1:Q:357:PHE:CZ	2.55	0.42
1:R:205:ILE:HB	1:R:206:PRO:CD	2.49	0.42
1:T:291:SER:OG	1:T:292:THR:N	2.52	0.42
1:T:351:PRO:O	1:T:355:LEU:HG	2.19	0.42
1:D:28:LEU:O	1:D:29:ILE:C	2.63	0.42
1:F:297:TRP:O	1:F:298:GLU:HB3	2.20	0.42
1:I:273:PHE:HB3	1:I:357:PHE:CZ	2.55	0.42
1:J:120:PHE:HE2	1:J:178:VAL:HG13	1.84	0.42
1:K:33:GLU:O	1:K:36:GLN:HB2	2.20	0.42
1:K:79:VAL:C	1:K:81:PRO:HD2	2.44	0.42
1:K:99:PHE:N	1:K:100:PRO:CD	2.83	0.42
1:K:359:ARG:HG3	1:T:399:LEU:O	2.19	0.42
1:L:356:GLU:HG3	1:L:359:ARG:HH21	1.83	0.42
1:M:184:ILE:HD13	1:M:184:ILE:HG21	1.66	0.42
1:O:410:LYS:HD3	1:O:410:LYS:HA	1.95	0.42
1:O:418:SER:O	1:O:422:VAL:HG23	2.20	0.42
1:Q:194:PHE:CD1	1:Q:207:ILE:HG12	2.55	0.42
1:R:430:ALA:O	1:R:431:VAL:HB	2.19	0.42
1:S:150:LEU:O	1:S:151:TYR:C	2.62	0.42
1:S:278:ARG:HD2	1:S:374:TYR:CZ	2.55	0.42
1:A:1:MSE:CE	1:A:4:GLN:HB2	2.49	0.42
1:A:408:THR:O	1:A:408:THR:HG23	2.20	0.42
1:D:350:TYR:N	1:D:351:PRO:CD	2.83	0.42
1:E:221:ARG:HB3	1:E:223:TYR:CE2	2.55	0.42
1:J:269:LEU:HD22	1:J:273:PHE:CE1	2.55	0.42
1:K:184:ILE:HD11	1:M:377:ASN:ND2	2.35	0.42
1:L:61:THR:O	1:L:61:THR:OG1	2.37	0.42
1:L:205:ILE:HB	1:L:206:PRO:HD3	2.02	0.42
1:M:99:PHE:CE1	1:M:103:ASN:ND2	2.88	0.42
1:M:267:ASP:OD1	1:M:267:ASP:N	2.51	0.42
1:O:231:TYR:O	1:O:232:ASP:C	2.61	0.42
1:Q:65:ASN:O	1:Q:69:ARG:HG3	2.19	0.42
1:R:251:LEU:HD23	1:R:251:LEU:HA	1.94	0.42
1:R:375:SER:CB	1:T:117:SER:HA	2.49	0.42
1:T:169:ASN:HA	1:T:172:ILE:HG12	2.02	0.42
1:A:152:VAL:O	1:A:153:SER:C	2.63	0.41
1:B:114:ASP:OD1	1:J:290:SER:OG	2.34	0.41
1:B:144:ILE:O	1:B:148:VAL:HG23	2.20	0.41
1:G:109:LYS:N	1:G:110:PRO:CD	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:56:GLU:O	1:H:57:ILE:C	2.63	0.41
1:I:99:PHE:HB3	1:I:100:PRO:HD3	2.02	0.41
1:I:180:VAL:O	1:I:184:ILE:HG23	2.20	0.41
1:J:61:THR:O	1:J:61:THR:OG1	2.34	0.41
1:K:281:MSE:O	1:K:282:ILE:C	2.61	0.41
1:Q:3:LEU:O	1:Q:3:LEU:HD23	2.20	0.41
1:Q:264:SER:O	1:Q:265:LEU:C	2.62	0.41
1:S:107:GLN:NE2	1:S:170:GLN:NE2	2.67	0.41
1:T:401:TYR:CE2	1:T:412:ARG:HG3	2.55	0.41
1:C:137:ARG:HB2	1:C:137:ARG:CZ	2.50	0.41
1:E:68:ARG:O	1:E:72:TRP:N	2.43	0.41
1:E:408:THR:O	1:E:408:THR:OG1	2.30	0.41
1:J:231:TYR:CZ	1:J:235:LEU:HD11	2.56	0.41
1:K:136:ARG:HA	1:K:136:ARG:HD2	1.80	0.41
1:K:163:GLU:C	1:K:165:GLN:H	2.27	0.41
1:K:278:ARG:HD2	1:K:374:TYR:CZ	2.55	0.41
1:L:278:ARG:HB2	1:L:374:TYR:CE2	2.55	0.41
1:L:424:LEU:O	1:L:424:LEU:HD23	2.20	0.41
1:M:208:LEU:HD23	1:M:208:LEU:HA	1.92	0.41
1:O:176:VAL:O	1:O:177:ASN:C	2.62	0.41
1:P:86:ASP:CB	1:P:135:LEU:HD22	2.51	0.41
1:Q:410:LYS:C	1:Q:412:ARG:N	2.78	0.41
1:S:208:LEU:HD23	1:S:208:LEU:HA	1.93	0.41
1:C:421:VAL:HG21	1:D:262:CYS:SG	2.60	0.41
1:D:136:ARG:HA	1:D:136:ARG:HD2	1.88	0.41
1:D:255:LEU:HD12	1:D:255:LEU:HA	1.98	0.41
1:E:2:PRO:HB3	1:E:38:ARG:CD	2.50	0.41
1:F:269:LEU:HD11	1:F:350:TYR:CG	2.55	0.41
1:J:147:LEU:HD23	1:J:147:LEU:HA	1.92	0.41
1:M:401:TYR:OH	1:M:412:ARG:HG2	2.21	0.41
1:N:14:LEU:HD13	1:N:57:ILE:HG21	2.03	0.41
1:O:277:LEU:O	1:O:278:ARG:C	2.62	0.41
1:O:278:ARG:HD2	1:O:374:TYR:CZ	2.55	0.41
1:Q:240:PHE:O	1:Q:241:ASP:C	2.60	0.41
1:R:39:TYR:N	1:R:40:PRO:CD	2.83	0.41
1:T:86:ASP:OD1	1:T:86:ASP:N	2.53	0.41
1:C:66:THR:O	1:C:67:ARG:C	2.61	0.41
1:C:152:VAL:HG12	1:C:153:SER:N	2.34	0.41
1:C:251:LEU:HD22	1:C:255:LEU:HD22	2.02	0.41
1:C:410:LYS:O	1:C:412:ARG:N	2.53	0.41
1:D:286:SER:HB3	1:F:116:LYS:NZ	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:6:LEU:O	1:E:9:ALA:HB3	2.20	0.41
1:F:296:ASN:OD1	1:F:296:ASN:N	2.53	0.41
1:G:198:PHE:CD1	1:G:204:ARG:HG2	2.54	0.41
1:G:261:ILE:HG22	1:G:262:CYS:N	2.35	0.41
1:H:251:LEU:HD22	1:H:255:LEU:CD2	2.44	0.41
1:J:408:THR:HG23	1:J:408:THR:O	2.19	0.41
1:K:342:LEU:HA	1:K:345:ILE:HG22	2.01	0.41
1:L:266:ASP:OD1	1:L:266:ASP:N	2.53	0.41
1:Q:90:VAL:CG2	1:Q:142:GLU:HG2	2.51	0.41
1:R:116:LYS:O	1:R:117:SER:C	2.63	0.41
1:A:136:ARG:HA	1:A:136:ARG:HD2	1.87	0.41
1:A:203:THR:O	1:A:206:PRO:HD2	2.20	0.41
1:B:25:LEU:CD2	1:B:74:ALA:HB1	2.50	0.41
1:B:208:LEU:HD23	1:B:208:LEU:HA	1.91	0.41
1:B:363:LEU:O	1:B:364:TYR:C	2.62	0.41
1:E:10:LEU:HA	1:E:13:VAL:HG12	2.02	0.41
1:E:62:PRO:HG2	1:E:64:ASN:CG	2.46	0.41
1:F:239:GLU:C	1:F:278:ARG:NH1	2.78	0.41
1:F:386:ASP:C	1:F:388:LEU:H	2.29	0.41
1:G:154:LYS:O	1:G:168:ARG:NH1	2.54	0.41
1:G:348:ALA:O	1:G:349:LEU:CB	2.65	0.41
1:I:209:SER:HA	1:I:249:TYR:CE1	2.56	0.41
1:I:414:THR:C	1:I:416:LEU:H	2.28	0.41
1:K:35:TYR:CD1	1:K:35:TYR:C	2.98	0.41
1:M:47:SER:O	1:M:48:GLN:C	2.63	0.41
1:M:208:LEU:HD12	1:M:246:LEU:HD11	2.03	0.41
1:N:80:ILE:HG23	1:N:81:PRO:CD	2.50	0.41
1:N:99:PHE:CD1	1:N:99:PHE:C	2.98	0.41
1:P:350:TYR:N	1:P:351:PRO:CD	2.83	0.41
1:A:65:ASN:HD21	1:A:68:ARG:HG3	1.86	0.41
1:A:152:VAL:CG1	1:A:203:THR:HG22	2.51	0.41
1:A:285:THR:CG2	1:I:173:GLU:HG2	2.51	0.41
1:B:7:VAL:O	1:B:8:LYS:C	2.63	0.41
1:B:276:TYR:CD2	1:B:276:TYR:C	2.98	0.41
1:G:281:MSE:SE	1:G:376:PHE:HB2	2.71	0.41
1:H:261:ILE:C	1:H:263:ASN:N	2.77	0.41
1:H:404:GLU:H	1:H:404:GLU:CD	2.28	0.41
1:L:180:VAL:O	1:L:181:HIS:C	2.62	0.41
1:N:130:GLU:HG2	1:N:130:GLU:O	2.19	0.41
1:O:282:ILE:O	1:O:282:ILE:HG23	2.19	0.41
1:Q:180:VAL:HG12	1:Q:181:HIS:N	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:190:LEU:HG	1:S:194:PHE:CE2	2.55	0.41
1:S:254:ILE:O	1:S:257:ILE:HG22	2.20	0.41
1:T:367:LYS:C	1:T:368:HIS:CD2	2.98	0.41
1:B:401:TYR:HB3	1:B:405:THR:OG1	2.21	0.41
1:C:299:VAL:CG1	1:C:300:PHE:N	2.83	0.41
1:D:70:ILE:HG12	1:D:111:VAL:HG21	2.03	0.41
1:D:235:LEU:O	1:D:239:GLU:CG	2.68	0.41
1:E:97:ILE:O	1:E:100:PRO:HG2	2.21	0.41
1:F:66:THR:O	1:F:69:ARG:N	2.53	0.41
1:F:201:PRO:HB2	1:F:202:PRO:HD3	2.02	0.41
1:F:225:ILE:HB	1:F:226:PRO:HD3	2.03	0.41
1:G:181:HIS:O	1:G:185:GLN:HG3	2.20	0.41
1:H:194:PHE:CE1	1:H:207:ILE:HG23	2.55	0.41
1:I:190:LEU:HD12	1:I:190:LEU:HA	1.81	0.41
1:I:192:SER:O	1:I:195:CYS:HB2	2.20	0.41
1:I:215:ILE:O	1:I:216:ARG:C	2.63	0.41
1:I:348:ALA:O	1:I:349:LEU:CB	2.68	0.41
1:N:254:ILE:HD11	1:N:272:LEU:HD21	2.02	0.41
1:N:348:ALA:O	1:N:349:LEU:CB	2.65	0.41
1:P:201:PRO:HB3	1:P:300:PHE:HB2	2.02	0.41
1:Q:108:LEU:HD21	1:S:303:PHE:HB2	2.03	0.41
1:B:35:TYR:CE1	1:B:82:LEU:HG	2.56	0.41
1:E:275:ILE:O	1:E:276:TYR:C	2.63	0.41
1:F:91:GLY:O	1:F:92:GLU:C	2.64	0.41
1:G:413:TRP:O	1:G:416:LEU:HB2	2.21	0.41
1:H:25:LEU:O	1:H:27:GLU:N	2.53	0.41
1:H:62:PRO:HG2	1:H:64:ASN:ND2	2.36	0.41
1:H:131:TRP:HZ3	1:H:139:CYS:SG	2.44	0.41
1:K:65:ASN:HD21	1:K:68:ARG:HG3	1.86	0.41
1:L:282:ILE:CD1	1:L:288:PHE:CZ	2.96	0.41
1:M:90:VAL:O	1:M:90:VAL:HG23	2.20	0.41
1:P:217:ARG:HG2	1:P:217:ARG:NH1	2.35	0.41
1:P:225:ILE:O	1:P:226:PRO:C	2.60	0.41
1:P:380:LEU:HB2	1:R:184:ILE:HD11	2.01	0.41
1:R:51:ARG:HG2	1:R:83:LEU:HD13	2.02	0.41
1:R:220:PRO:HB2	1:R:221:ARG:HG2	2.03	0.41
1:T:342:LEU:HA	1:T:345:ILE:HG22	2.01	0.41
1:C:53:ILE:O	1:C:57:ILE:HG13	2.20	0.41
1:C:410:LYS:C	1:C:412:ARG:N	2.77	0.41
1:D:208:LEU:HA	1:D:208:LEU:HD23	1.85	0.41
1:E:8:LYS:O	1:E:12:ASN:OD1	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:154:LYS:HG2	1:E:171:THR:HG21	2.03	0.41
1:E:242:THR:O	1:E:242:THR:CG2	2.68	0.41
1:E:360:ASP:OD1	1:E:360:ASP:C	2.62	0.41
1:F:32:VAL:O	1:F:35:TYR:HB3	2.20	0.41
1:F:65:ASN:ND2	1:F:68:ARG:HG3	2.35	0.41
1:F:175:LEU:HD23	1:F:175:LEU:HA	1.85	0.41
1:F:376:PHE:O	1:F:376:PHE:CG	2.72	0.41
1:G:1:MSE:HE1	1:G:8:LYS:HE2	2.03	0.41
1:H:3:LEU:O	1:H:7:VAL:HG23	2.21	0.41
1:H:32:VAL:O	1:H:36:GLN:HG3	2.21	0.41
1:I:233:LEU:HA	1:I:233:LEU:HD12	1.78	0.41
1:J:182:TYR:O	1:J:185:GLN:N	2.52	0.41
1:K:123:LEU:O	1:K:124:ILE:HD13	2.21	0.41
1:L:251:LEU:HG	1:L:279:PHE:CE2	2.56	0.41
1:N:33:GLU:O	1:N:36:GLN:N	2.54	0.41
1:N:76:LEU:O	1:N:80:ILE:HG22	2.21	0.41
1:N:86:ASP:HB3	1:N:135:LEU:CD2	2.51	0.41
1:N:191:SER:HB3	1:N:211:MSE:HE2	2.02	0.41
1:N:394:ALA:HB3	1:O:389:LEU:HG	2.03	0.41
1:P:225:ILE:HB	1:P:226:PRO:HD3	2.03	0.41
1:P:261:ILE:C	1:P:263:ASN:H	2.28	0.41
1:P:297:TRP:O	1:P:298:GLU:HB3	2.21	0.41
1:Q:254:ILE:HG21	1:Q:254:ILE:HD13	1.78	0.41
1:S:6:LEU:HD23	1:S:6:LEU:C	2.45	0.41
1:T:49:LYS:O	1:T:53:ILE:HG12	2.21	0.41
1:T:251:LEU:HG	1:T:279:PHE:CE2	2.56	0.41
1:D:3:LEU:HD23	1:D:7:VAL:HG23	2.03	0.41
1:D:8:LYS:O	1:D:9:ALA:C	2.64	0.41
1:F:99:PHE:HE1	1:F:103:ASN:HD22	1.69	0.41
1:F:136:ARG:HA	1:F:136:ARG:HD2	1.86	0.41
1:F:399:LEU:HD21	1:G:355:LEU:HD22	2.02	0.41
1:F:415:ARG:O	1:F:419:ILE:HG23	2.21	0.41
1:H:345:ILE:O	1:H:348:ALA:O	2.39	0.41
1:I:294:SER:O	1:I:295:GLY:C	2.63	0.41
1:I:363:LEU:O	1:I:363:LEU:CD2	2.68	0.41
1:J:153:SER:OG	1:J:154:LYS:N	2.54	0.41
1:M:201:PRO:HB3	1:M:300:PHE:HB2	2.03	0.41
1:M:204:ARG:CZ	1:M:297:TRP:CZ2	3.04	0.41
1:N:139:CYS:O	1:N:143:THR:OG1	2.38	0.41
1:O:98:PHE:HD1	1:O:115:LEU:HD21	1.85	0.41
1:Q:262:CYS:SG	1:R:421:VAL:HG21	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:107:GLN:O	1:S:108:LEU:HD23	2.21	0.41
1:A:200:ASN:HA	1:A:201:PRO:HD2	1.90	0.40
1:B:347:TYR:C	1:B:348:ALA:O	2.62	0.40
1:E:343:PHE:C	1:E:343:PHE:CD1	2.99	0.40
1:F:277:LEU:HD23	1:F:277:LEU:O	2.21	0.40
1:H:50:ILE:O	1:H:54:LEU:HD22	2.21	0.40
1:J:194:PHE:CD1	1:J:207:ILE:HG23	2.56	0.40
1:L:281:MSE:SE	1:L:377:ASN:H	2.54	0.40
1:N:1:MSE:HE2	1:N:4:GLN:CB	2.50	0.40
1:N:69:ARG:O	1:N:70:ILE:C	2.63	0.40
1:O:65:ASN:ND2	1:O:68:ARG:HG3	2.35	0.40
1:Q:245:ILE:O	1:Q:249:TYR:HD2	2.03	0.40
1:R:101:PHE:CD1	1:R:101:PHE:C	2.99	0.40
1:B:28:LEU:O	1:B:32:VAL:HG23	2.22	0.40
1:C:235:LEU:O	1:C:239:GLU:HG2	2.20	0.40
1:D:65:ASN:ND2	1:D:68:ARG:CG	2.84	0.40
1:D:352:ILE:HB	1:D:406:GLU:OE1	2.21	0.40
1:H:237:CYS:SG	1:H:246:LEU:HD21	2.61	0.40
1:J:119:LEU:O	1:J:123:LEU:HD22	2.22	0.40
1:J:430:ALA:O	1:J:431:VAL:CB	2.69	0.40
1:K:51:ARG:HG2	1:K:83:LEU:HD13	2.03	0.40
1:K:243:SER:OG	1:K:302:ASP:OD2	2.38	0.40
1:M:271:ARG:O	1:M:275:ILE:HG13	2.22	0.40
1:M:342:LEU:HD12	1:M:342:LEU:HA	1.85	0.40
1:M:410:LYS:C	1:M:412:ARG:H	2.29	0.40
1:N:89:ALA:O	1:N:93:TRP:HD1	2.04	0.40
1:N:137:ARG:HG2	1:N:141:GLU:OE1	2.21	0.40
1:N:366:SER:C	1:N:368:HIS:H	2.29	0.40
1:O:107:GLN:HE22	1:O:170:GLN:NE2	2.18	0.40
1:Q:109:LYS:N	1:Q:110:PRO:CD	2.84	0.40
1:Q:208:LEU:HD23	1:Q:208:LEU:HA	1.95	0.40
1:R:35:TYR:CD1	1:R:35:TYR:C	2.99	0.40
1:R:208:LEU:O	1:R:212:VAL:HG13	2.22	0.40
1:S:402:THR:O	1:S:403:ALA:C	2.64	0.40
1:T:66:THR:O	1:T:67:ARG:C	2.63	0.40
1:T:273:PHE:HB3	1:T:357:PHE:CD2	2.56	0.40
1:A:299:VAL:HG12	1:A:300:PHE:N	2.36	0.40
1:E:254:ILE:CG1	1:E:255:LEU:N	2.82	0.40
1:G:144:ILE:HG23	1:G:145:THR:N	2.36	0.40
1:G:238:ALA:O	1:G:278:ARG:NH1	2.49	0.40
1:J:80:ILE:HA	1:J:83:LEU:HG	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:363:LEU:O	1:M:364:TYR:C	2.65	0.40
1:N:49:LYS:O	1:N:53:ILE:HG12	2.20	0.40
1:Q:300:PHE:CD1	1:Q:300:PHE:C	2.98	0.40
1:S:3:LEU:O	1:S:7:VAL:HG23	2.22	0.40
1:S:84:ILE:O	1:S:85:LEU:HD12	2.21	0.40
1:T:63:PHE:CE1	1:T:69:ARG:HA	2.56	0.40
1:A:104:SER:HA	1:A:105:PRO:HD3	1.90	0.40
1:A:106:THR:O	1:A:108:LEU:N	2.53	0.40
1:D:208:LEU:HD21	1:D:234:VAL:HG22	2.03	0.40
1:E:215:ILE:CG2	1:E:256:MSE:HB3	2.52	0.40
1:E:217:ARG:O	1:E:218:GLN:C	2.63	0.40
1:E:341:GLN:O	1:E:345:ILE:HG22	2.22	0.40
1:F:270:TYR:HB3	1:F:370:PHE:CE2	2.56	0.40
1:F:283:ASP:HA	1:F:284:PRO:HD3	1.96	0.40
1:G:299:VAL:CG1	1:G:301:HIS:CE1	2.96	0.40
1:H:208:LEU:O	1:H:209:SER:C	2.65	0.40
1:H:247:LEU:HD23	1:H:247:LEU:HA	1.95	0.40
1:H:248:SER:O	1:H:252:SER:OG	2.38	0.40
1:I:156:ILE:HD11	1:I:203:THR:HG22	2.02	0.40
1:J:354:PHE:CZ	1:J:358:LEU:HD11	2.56	0.40
1:K:396:SER:O	1:K:398:PHE:N	2.55	0.40
1:M:347:TYR:O	1:M:351:PRO:HB3	2.20	0.40
1:N:94:TRP:CG	1:N:146:ARG:HD3	2.57	0.40
1:N:118:ILE:O	1:N:122:ILE:HG13	2.22	0.40
1:P:265:LEU:O	1:P:269:LEU:HB2	2.22	0.40
1:Q:57:ILE:O	1:Q:57:ILE:HG22	2.20	0.40
1:S:209:SER:HA	1:S:249:TYR:CE1	2.57	0.40
1:A:247:LEU:CD1	1:A:288:PHE:CD1	3.03	0.40
1:D:414:THR:O	1:D:415:ARG:C	2.65	0.40
1:E:237:CYS:O	1:E:241:ASP:HB2	2.21	0.40
1:G:380:LEU:HD12	1:G:380:LEU:HA	1.83	0.40
1:H:80:ILE:HD12	1:H:93:TRP:CH2	2.57	0.40
1:J:3:LEU:HD12	1:J:46:ASN:CG	2.47	0.40
1:J:99:PHE:O	1:J:103:ASN:HB2	2.20	0.40
1:K:208:LEU:O	1:K:209:SER:C	2.65	0.40
1:L:208:LEU:O	1:L:209:SER:C	2.64	0.40
1:N:297:TRP:O	1:N:298:GLU:HB3	2.20	0.40
1:O:207:ILE:O	1:O:208:LEU:C	2.65	0.40
1:P:62:PRO:HG2	1:P:64:ASN:ND2	2.36	0.40
1:P:208:LEU:HD23	1:P:208:LEU:HA	1.87	0.40
1:P:282:ILE:HG23	1:P:282:ILE:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:230:PHE:O	1:S:234:VAL:HG23	2.22	0.40
1:T:244:PRO:HD2	1:T:302:ASP:OD2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	395/434 (91%)	331 (84%)	45 (11%)	19 (5%)	2	12
1	B	383/434 (88%)	333 (87%)	33 (9%)	17 (4%)	2	13
1	C	383/434 (88%)	335 (88%)	36 (9%)	12 (3%)	3	20
1	D	383/434 (88%)	333 (87%)	41 (11%)	9 (2%)	5	25
1	E	383/434 (88%)	336 (88%)	35 (9%)	12 (3%)	3	20
1	F	383/434 (88%)	347 (91%)	29 (8%)	7 (2%)	6	29
1	G	383/434 (88%)	325 (85%)	48 (12%)	10 (3%)	4	23
1	H	383/434 (88%)	320 (84%)	46 (12%)	17 (4%)	2	13
1	I	383/434 (88%)	328 (86%)	39 (10%)	16 (4%)	2	14
1	J	383/434 (88%)	314 (82%)	55 (14%)	14 (4%)	2	17
1	K	395/434 (91%)	346 (88%)	36 (9%)	13 (3%)	3	19
1	L	383/434 (88%)	327 (85%)	47 (12%)	9 (2%)	5	25
1	M	383/434 (88%)	327 (85%)	46 (12%)	10 (3%)	4	23
1	N	383/434 (88%)	323 (84%)	50 (13%)	10 (3%)	4	23
1	O	383/434 (88%)	331 (86%)	42 (11%)	10 (3%)	4	23
1	P	383/434 (88%)	342 (89%)	31 (8%)	10 (3%)	4	23
1	Q	383/434 (88%)	308 (80%)	63 (16%)	12 (3%)	3	20
1	R	383/434 (88%)	334 (87%)	41 (11%)	8 (2%)	5	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	S	383/434 (88%)	315 (82%)	58 (15%)	10 (3%)	4	23
1	T	383/434 (88%)	343 (90%)	35 (9%)	5 (1%)	9	35
All	All	7684/8680 (88%)	6598 (86%)	856 (11%)	230 (3%)	3	20

All (230) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1	MSE
1	A	64	ASN
1	A	164	SER
1	A	165	GLN
1	A	262	CYS
1	A	298	GLU
1	A	328	SER
1	A	397	ASN
1	A	409	ASP
1	B	165	GLN
1	B	261	ILE
1	B	359	ARG
1	B	397	ASN
1	C	293	ALA
1	C	359	ARG
1	E	135	LEU
1	E	293	ALA
1	G	2	PRO
1	H	130	GLU
1	H	262	CYS
1	H	282	ILE
1	H	293	ALA
1	H	409	ASP
1	I	2	PRO
1	I	293	ALA
1	I	409	ASP
1	K	295	GLY
1	K	409	ASP
1	K	415	ARG
1	L	26	THR
1	L	262	CYS
1	L	349	LEU
1	L	397	ASN
1	M	135	LEU

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Mol	Chain	Res	Type
1	N	293	ALA
1	O	156	ILE
1	O	157	GLU
1	O	223	TYR
1	P	157	GLU
1	P	159	LEU
1	P	262	CYS
1	Q	48	GLN
1	Q	159	LEU
1	Q	298	GLU
1	R	262	CYS
1	R	349	LEU
1	R	409	ASP
1	S	130	GLU
1	S	241	ASP
1	A	294	SER
1	B	10	LEU
1	B	26	THR
1	B	349	LEU
1	C	262	CYS
1	C	295	GLY
1	C	397	ASN
1	D	2	PRO
1	D	133	GLY
1	D	157	GLU
1	E	261	ILE
1	E	295	GLY
1	F	92	GLU
1	F	295	GLY
1	F	369	ASN
1	F	387	GLY
1	G	26	THR
1	G	266	ASP
1	G	295	GLY
1	G	298	GLU
1	H	26	THR
1	H	62	PRO
1	H	415	ARG
1	I	62	PRO
1	I	157	GLU
1	I	159	LEU
1	I	349	LEU

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Mol	Chain	Res	Type
1	I	415	ARG
1	J	60	LYS
1	J	181	HIS
1	J	294	SER
1	J	367	LYS
1	J	397	ASN
1	K	2	PRO
1	K	165	GLN
1	K	298	GLU
1	L	130	GLU
1	M	62	PRO
1	M	218	GLN
1	M	261	ILE
1	M	298	GLU
1	N	159	LEU
1	O	2	PRO
1	O	261	ILE
1	O	298	GLU
1	O	349	LEU
1	P	62	PRO
1	P	295	GLY
1	P	396	SER
1	Q	47	SER
1	Q	295	GLY
1	Q	382	SER
1	Q	409	ASP
1	R	62	PRO
1	S	261	ILE
1	S	294	SER
1	T	261	ILE
1	T	397	ASN
1	T	415	ARG
1	A	74	ALA
1	A	367	LYS
1	B	2	PRO
1	B	40	PRO
1	B	103	ASN
1	B	383	THR
1	C	159	LEU
1	C	369	ASN
1	C	411	SER
1	D	64	ASN

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Mol	Chain	Res	Type
1	D	261	ILE
1	D	415	ARG
1	E	62	PRO
1	E	119	LEU
1	E	130	GLU
1	G	397	ASN
1	H	2	PRO
1	H	107	GLN
1	H	294	SER
1	H	367	LYS
1	H	413	TRP
1	I	262	CYS
1	I	302	ASP
1	I	383	THR
1	J	92	GLU
1	J	159	LEU
1	J	256	MSE
1	J	262	CYS
1	J	383	THR
1	J	409	ASP
1	K	128	GLU
1	K	154	LYS
1	K	369	ASN
1	L	159	LEU
1	M	107	GLN
1	M	130	GLU
1	M	159	LEU
1	M	409	ASP
1	N	62	PRO
1	N	135	LEU
1	N	261	ILE
1	N	298	GLU
1	O	26	THR
1	O	130	GLU
1	P	298	GLU
1	P	367	LYS
1	P	415	ARG
1	Q	2	PRO
1	Q	383	THR
1	R	2	PRO
1	S	409	ASP
1	T	295	GLY

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Mol	Chain	Res	Type
1	A	2	PRO
1	A	358	LEU
1	B	62	PRO
1	B	157	GLU
1	B	348	ALA
1	C	62	PRO
1	C	367	LYS
1	D	293	ALA
1	E	101	PHE
1	E	409	ASP
1	G	62	PRO
1	H	77	LYS
1	H	195	CYS
1	I	47	SER
1	I	107	GLN
1	J	382	SER
1	K	329	SER
1	K	397	ASN
1	L	409	ASP
1	L	411	SER
1	M	302	ASP
1	N	181	HIS
1	N	241	ASP
1	O	293	ALA
1	P	2	PRO
1	Q	62	PRO
1	S	107	GLN
1	S	189	GLU
1	S	258	LEU
1	A	62	PRO
1	A	166	GLU
1	B	70	ILE
1	B	298	GLU
1	C	219	GLY
1	D	243	SER
1	F	367	LYS
1	G	157	GLU
1	I	154	LYS
1	J	349	LEU
1	K	62	PRO
1	L	359	ARG
1	N	11	TRP

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Mol	Chain	Res	Type
1	R	298	GLU
1	S	119	LEU
1	A	293	ALA
1	B	159	LEU
1	D	62	PRO
1	E	165	GLN
1	H	261	ILE
1	I	158	ASN
1	I	295	GLY
1	J	2	PRO
1	K	331	PRO
1	N	40	PRO
1	S	202	PRO
1	E	118	ILE
1	F	62	PRO
1	G	152	VAL
1	C	261	ILE
1	E	2	PRO
1	F	261	ILE
1	G	148	VAL
1	Q	299	VAL
1	R	295	GLY
1	T	2	PRO
1	A	118	ILE
1	A	176	VAL
1	H	160	GLY
1	Q	261	ILE
1	R	282	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	361/398 (91%)	303 (84%)	58 (16%)	2 12
1	B	352/398 (88%)	298 (85%)	54 (15%)	3 13
1	C	352/398 (88%)	298 (85%)	54 (15%)	3 13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	352/398 (88%)	301 (86%)	51 (14%)	3	14
1	E	352/398 (88%)	295 (84%)	57 (16%)	2	11
1	F	352/398 (88%)	307 (87%)	45 (13%)	4	18
1	G	352/398 (88%)	307 (87%)	45 (13%)	4	18
1	H	352/398 (88%)	296 (84%)	56 (16%)	2	12
1	I	352/398 (88%)	295 (84%)	57 (16%)	2	11
1	J	352/398 (88%)	301 (86%)	51 (14%)	3	14
1	K	361/398 (91%)	307 (85%)	54 (15%)	3	13
1	L	352/398 (88%)	302 (86%)	50 (14%)	3	14
1	M	352/398 (88%)	303 (86%)	49 (14%)	3	15
1	N	352/398 (88%)	297 (84%)	55 (16%)	2	12
1	O	352/398 (88%)	288 (82%)	64 (18%)	2	8
1	P	352/398 (88%)	293 (83%)	59 (17%)	2	11
1	Q	352/398 (88%)	295 (84%)	57 (16%)	2	11
1	R	352/398 (88%)	311 (88%)	41 (12%)	5	21
1	S	352/398 (88%)	307 (87%)	45 (13%)	4	18
1	T	352/398 (88%)	302 (86%)	50 (14%)	3	14
All	All	7058/7960 (89%)	6006 (85%)	1052 (15%)	3	13

All (1052) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	SER
1	A	26	THR
1	A	35	TYR
1	A	52	HIS
1	A	54	LEU
1	A	55	ASP
1	A	57	ILE
1	A	60	LYS
1	A	61	THR
1	A	63	PHE
1	A	64	ASN
1	A	66	THR
1	A	76	LEU
1	A	78	THR

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Mol	Chain	Res	Type
1	A	82	LEU
1	A	86	ASP
1	A	90	VAL
1	A	108	LEU
1	A	113	SER
1	A	115	LEU
1	A	119	LEU
1	A	123	LEU
1	A	129	ASP
1	A	134	ASP
1	A	143	THR
1	A	156	ILE
1	A	157	GLU
1	A	165	GLN
1	A	196	HIS
1	A	205	ILE
1	A	221	ARG
1	A	242	THR
1	A	251	LEU
1	A	254	ILE
1	A	255	LEU
1	A	258	LEU
1	A	259	SER
1	A	264	SER
1	A	265	LEU
1	A	266	ASP
1	A	268	SER
1	A	269	LEU
1	A	277	LEU
1	A	285	THR
1	A	286	SER
1	A	340	SER
1	A	345	ILE
1	A	363	LEU
1	A	375	SER
1	A	379	GLU
1	A	382	SER
1	A	383	THR
1	A	396	SER
1	A	404	GLU
1	A	405	THR
1	A	416	LEU

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Mol	Chain	Res	Type
1	A	424	LEU
1	A	428	LEU
1	B	1	MSE
1	B	4	GLN
1	B	6	LEU
1	B	10	LEU
1	B	13	VAL
1	B	26	THR
1	B	29	ILE
1	B	37	GLN
1	B	45	THR
1	B	52	HIS
1	B	54	LEU
1	B	60	LYS
1	B	61	THR
1	B	76	LEU
1	B	78	THR
1	B	82	LEU
1	B	85	LEU
1	B	99	PHE
1	B	108	LEU
1	B	115	LEU
1	B	119	LEU
1	B	123	LEU
1	B	154	LYS
1	B	156	ILE
1	B	172	ILE
1	B	177	ASN
1	B	180	VAL
1	B	184	ILE
1	B	191	SER
1	B	196	HIS
1	B	205	ILE
1	B	211	MSE
1	B	212	VAL
1	B	221	ARG
1	B	233	LEU
1	B	251	LEU
1	B	255	LEU
1	B	258	LEU
1	B	265	LEU
1	B	267	ASP

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Mol	Chain	Res	Type
1	B	269	LEU
1	B	277	LEU
1	B	285	THR
1	B	304	MSE
1	B	338	ASP
1	B	375	SER
1	B	379	GLU
1	B	383	THR
1	B	400	LYS
1	B	404	GLU
1	B	414	THR
1	B	418	SER
1	B	424	LEU
1	B	428	LEU
1	C	1	MSE
1	C	3	LEU
1	C	10	LEU
1	C	25	LEU
1	C	26	THR
1	C	29	ILE
1	C	34	SER
1	C	36	GLN
1	C	43	ASN
1	C	45	THR
1	C	52	HIS
1	C	54	LEU
1	C	60	LYS
1	C	61	THR
1	C	64	ASN
1	C	66	THR
1	C	70	ILE
1	C	76	LEU
1	C	82	LEU
1	C	85	LEU
1	C	106	THR
1	C	115	LEU
1	C	119	LEU
1	C	123	LEU
1	C	152	VAL
1	C	154	LYS
1	C	176	VAL
1	C	191	SER

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Mol	Chain	Res	Type
1	C	196	HIS
1	C	210	VAL
1	C	221	ARG
1	C	225	ILE
1	C	226	PRO
1	C	239	GLU
1	C	242	THR
1	C	251	LEU
1	C	254	ILE
1	C	255	LEU
1	C	258	LEU
1	C	265	LEU
1	C	267	ASP
1	C	269	LEU
1	C	285	THR
1	C	304	MSE
1	C	337	LEU
1	C	363	LEU
1	C	371	GLN
1	C	379	GLU
1	C	396	SER
1	C	400	LYS
1	C	404	GLU
1	C	416	LEU
1	C	424	LEU
1	C	428	LEU
1	D	1	MSE
1	D	13	VAL
1	D	26	THR
1	D	34	SER
1	D	36	GLN
1	D	45	THR
1	D	52	HIS
1	D	54	LEU
1	D	60	LYS
1	D	61	THR
1	D	64	ASN
1	D	66	THR
1	D	76	LEU
1	D	77	LYS
1	D	82	LEU
1	D	85	LEU

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Mol	Chain	Res	Type
1	D	90	VAL
1	D	100	PRO
1	D	115	LEU
1	D	119	LEU
1	D	123	LEU
1	D	128	GLU
1	D	184	ILE
1	D	191	SER
1	D	196	HIS
1	D	205	ILE
1	D	215	ILE
1	D	221	ARG
1	D	232	ASP
1	D	251	LEU
1	D	252	SER
1	D	254	ILE
1	D	255	LEU
1	D	257	ILE
1	D	259	SER
1	D	264	SER
1	D	265	LEU
1	D	268	SER
1	D	269	LEU
1	D	304	MSE
1	D	337	LEU
1	D	340	SER
1	D	363	LEU
1	D	375	SER
1	D	382	SER
1	D	391	ARG
1	D	404	GLU
1	D	412	ARG
1	D	424	LEU
1	D	428	LEU
1	D	431	VAL
1	E	1	MSE
1	E	3	LEU
1	E	10	LEU
1	E	13	VAL
1	E	26	THR
1	E	29	ILE
1	E	34	SER

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Mol	Chain	Res	Type
1	E	37	GLN
1	E	45	THR
1	E	54	LEU
1	E	60	LYS
1	E	64	ASN
1	E	66	THR
1	E	71	LEU
1	E	76	LEU
1	E	78	THR
1	E	82	LEU
1	E	108	LEU
1	E	115	LEU
1	E	119	LEU
1	E	123	LEU
1	E	128	GLU
1	E	136	ARG
1	E	154	LYS
1	E	156	ILE
1	E	172	ILE
1	E	191	SER
1	E	196	HIS
1	E	221	ARG
1	E	233	LEU
1	E	242	THR
1	E	251	LEU
1	E	252	SER
1	E	254	ILE
1	E	255	LEU
1	E	258	LEU
1	E	259	SER
1	E	264	SER
1	E	265	LEU
1	E	266	ASP
1	E	269	LEU
1	E	277	LEU
1	E	292	THR
1	E	304	MSE
1	E	341	GLN
1	E	345	ILE
1	E	363	LEU
1	E	375	SER
1	E	379	GLU

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Mol	Chain	Res	Type
1	E	396	SER
1	E	404	GLU
1	E	408	THR
1	E	412	ARG
1	E	414	THR
1	E	417	ASP
1	E	424	LEU
1	E	428	LEU
1	F	1	MSE
1	F	5	SER
1	F	10	LEU
1	F	26	THR
1	F	29	ILE
1	F	36	GLN
1	F	45	THR
1	F	48	GLN
1	F	52	HIS
1	F	54	LEU
1	F	60	LYS
1	F	76	LEU
1	F	77	LYS
1	F	82	LEU
1	F	88	GLN
1	F	108	LEU
1	F	115	LEU
1	F	119	LEU
1	F	123	LEU
1	F	124	ILE
1	F	154	LYS
1	F	184	ILE
1	F	192	SER
1	F	201	PRO
1	F	221	ARG
1	F	242	THR
1	F	245	ILE
1	F	251	LEU
1	F	252	SER
1	F	254	ILE
1	F	255	LEU
1	F	257	ILE
1	F	258	LEU
1	F	259	SER

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Mol	Chain	Res	Type
1	F	264	SER
1	F	267	ASP
1	F	268	SER
1	F	269	LEU
1	F	285	THR
1	F	302	ASP
1	F	304	MSE
1	F	337	LEU
1	F	366	SER
1	F	404	GLU
1	F	419	ILE
1	G	1	MSE
1	G	3	LEU
1	G	5	SER
1	G	26	THR
1	G	35	TYR
1	G	45	THR
1	G	54	LEU
1	G	57	ILE
1	G	76	LEU
1	G	82	LEU
1	G	90	VAL
1	G	95	ASP
1	G	108	LEU
1	G	115	LEU
1	G	119	LEU
1	G	123	LEU
1	G	134	ASP
1	G	136	ARG
1	G	176	VAL
1	G	184	ILE
1	G	215	ILE
1	G	232	ASP
1	G	245	ILE
1	G	251	LEU
1	G	254	ILE
1	G	255	LEU
1	G	257	ILE
1	G	258	LEU
1	G	259	SER
1	G	264	SER
1	G	266	ASP

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Mol	Chain	Res	Type
1	G	269	LEU
1	G	285	THR
1	G	290	SER
1	G	302	ASP
1	G	304	MSE
1	G	345	ILE
1	G	363	LEU
1	G	375	SER
1	G	382	SER
1	G	383	THR
1	G	396	SER
1	G	404	GLU
1	G	408	THR
1	G	424	LEU
1	H	5	SER
1	H	12	ASN
1	H	26	THR
1	H	35	TYR
1	H	45	THR
1	H	48	GLN
1	H	52	HIS
1	H	54	LEU
1	H	57	ILE
1	H	60	LYS
1	H	64	ASN
1	H	66	THR
1	H	76	LEU
1	H	78	THR
1	H	82	LEU
1	H	85	LEU
1	H	90	VAL
1	H	103	ASN
1	H	108	LEU
1	H	115	LEU
1	H	119	LEU
1	H	123	LEU
1	H	149	ASP
1	H	184	ILE
1	H	191	SER
1	H	199	LEU
1	H	201	PRO
1	H	209	SER

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Mol	Chain	Res	Type
1	H	221	ARG
1	H	233	LEU
1	H	242	THR
1	H	251	LEU
1	H	252	SER
1	H	254	ILE
1	H	255	LEU
1	H	258	LEU
1	H	265	LEU
1	H	266	ASP
1	H	267	ASP
1	H	269	LEU
1	H	277	LEU
1	H	280	SER
1	H	290	SER
1	H	299	VAL
1	H	304	MSE
1	H	341	GLN
1	H	371	GLN
1	H	391	ARG
1	H	396	SER
1	H	404	GLU
1	H	405	THR
1	H	408	THR
1	H	411	SER
1	H	416	LEU
1	H	424	LEU
1	H	428	LEU
1	I	1	MSE
1	I	3	LEU
1	I	26	THR
1	I	36	GLN
1	I	45	THR
1	I	48	GLN
1	I	54	LEU
1	I	55	ASP
1	I	57	ILE
1	I	60	LYS
1	I	61	THR
1	I	66	THR
1	I	76	LEU
1	I	78	THR

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Mol	Chain	Res	Type
1	I	82	LEU
1	I	88	GLN
1	I	109	LYS
1	I	115	LEU
1	I	119	LEU
1	I	123	LEU
1	I	129	ASP
1	I	134	ASP
1	I	154	LYS
1	I	184	ILE
1	I	191	SER
1	I	195	CYS
1	I	200	ASN
1	I	209	SER
1	I	221	ARG
1	I	232	ASP
1	I	233	LEU
1	I	242	THR
1	I	251	LEU
1	I	254	ILE
1	I	255	LEU
1	I	257	ILE
1	I	258	LEU
1	I	265	LEU
1	I	268	SER
1	I	269	LEU
1	I	277	LEU
1	I	286	SER
1	I	289	PRO
1	I	291	SER
1	I	304	MSE
1	I	337	LEU
1	I	341	GLN
1	I	363	LEU
1	I	375	SER
1	I	396	SER
1	I	400	LYS
1	I	404	GLU
1	I	408	THR
1	I	416	LEU
1	I	418	SER
1	I	424	LEU

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Mol	Chain	Res	Type
1	I	428	LEU
1	J	13	VAL
1	J	14	LEU
1	J	26	THR
1	J	35	TYR
1	J	36	GLN
1	J	41	LYS
1	J	54	LEU
1	J	60	LYS
1	J	61	THR
1	J	66	THR
1	J	76	LEU
1	J	78	THR
1	J	79	VAL
1	J	82	LEU
1	J	83	LEU
1	J	103	ASN
1	J	115	LEU
1	J	119	LEU
1	J	123	LEU
1	J	145	THR
1	J	156	ILE
1	J	176	VAL
1	J	199	LEU
1	J	221	ARG
1	J	233	LEU
1	J	242	THR
1	J	248	SER
1	J	251	LEU
1	J	252	SER
1	J	254	ILE
1	J	255	LEU
1	J	265	LEU
1	J	267	ASP
1	J	268	SER
1	J	269	LEU
1	J	277	LEU
1	J	286	SER
1	J	302	ASP
1	J	304	MSE
1	J	337	LEU
1	J	341	GLN

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Mol	Chain	Res	Type
1	J	363	LEU
1	J	375	SER
1	J	379	GLU
1	J	391	ARG
1	J	396	SER
1	J	404	GLU
1	J	416	LEU
1	J	424	LEU
1	J	427	SER
1	J	428	LEU
1	K	1	MSE
1	K	3	LEU
1	K	4	GLN
1	K	13	VAL
1	K	26	THR
1	K	29	ILE
1	K	34	SER
1	K	36	GLN
1	K	45	THR
1	K	54	LEU
1	K	60	LYS
1	K	61	THR
1	K	70	ILE
1	K	77	LYS
1	K	78	THR
1	K	82	LEU
1	K	85	LEU
1	K	92	GLU
1	K	108	LEU
1	K	115	LEU
1	K	119	LEU
1	K	134	ASP
1	K	154	LYS
1	K	157	GLU
1	K	158	ASN
1	K	159	LEU
1	K	165	GLN
1	K	174	CYS
1	K	191	SER
1	K	196	HIS
1	K	209	SER
1	K	212	VAL

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Mol	Chain	Res	Type
1	K	215	ILE
1	K	221	ARG
1	K	227	GLN
1	K	233	LEU
1	K	245	ILE
1	K	251	LEU
1	K	254	ILE
1	K	255	LEU
1	K	265	LEU
1	K	266	ASP
1	K	269	LEU
1	K	282	ILE
1	K	285	THR
1	K	286	SER
1	K	302	ASP
1	K	304	MSE
1	K	305	SER
1	K	337	LEU
1	K	340	SER
1	K	363	LEU
1	K	404	GLU
1	K	428	LEU
1	L	1	MSE
1	L	13	VAL
1	L	26	THR
1	L	29	ILE
1	L	34	SER
1	L	37	GLN
1	L	45	THR
1	L	52	HIS
1	L	54	LEU
1	L	55	ASP
1	L	57	ILE
1	L	60	LYS
1	L	61	THR
1	L	66	THR
1	L	76	LEU
1	L	82	LEU
1	L	108	LEU
1	L	115	LEU
1	L	119	LEU
1	L	123	LEU

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Mol	Chain	Res	Type
1	L	137	ARG
1	L	145	THR
1	L	154	LYS
1	L	156	ILE
1	L	176	VAL
1	L	184	ILE
1	L	212	VAL
1	L	221	ARG
1	L	233	LEU
1	L	242	THR
1	L	248	SER
1	L	251	LEU
1	L	254	ILE
1	L	255	LEU
1	L	257	ILE
1	L	265	LEU
1	L	266	ASP
1	L	267	ASP
1	L	268	SER
1	L	269	LEU
1	L	290	SER
1	L	304	MSE
1	L	363	LEU
1	L	375	SER
1	L	383	THR
1	L	404	GLU
1	L	412	ARG
1	L	424	LEU
1	L	426	ASN
1	L	428	LEU
1	M	1	MSE
1	M	26	THR
1	M	36	GLN
1	M	49	LYS
1	M	52	HIS
1	M	54	LEU
1	M	57	ILE
1	M	64	ASN
1	M	66	THR
1	M	71	LEU
1	M	76	LEU
1	M	82	LEU

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Mol	Chain	Res	Type
1	M	90	VAL
1	M	106	THR
1	M	115	LEU
1	M	117	SER
1	M	119	LEU
1	M	123	LEU
1	M	134	ASP
1	M	154	LYS
1	M	196	HIS
1	M	206	PRO
1	M	217	ARG
1	M	221	ARG
1	M	233	LEU
1	M	248	SER
1	M	251	LEU
1	M	252	SER
1	M	254	ILE
1	M	255	LEU
1	M	257	ILE
1	M	258	LEU
1	M	265	LEU
1	M	267	ASP
1	M	269	LEU
1	M	277	LEU
1	M	286	SER
1	M	291	SER
1	M	304	MSE
1	M	341	GLN
1	M	345	ILE
1	M	363	LEU
1	M	369	ASN
1	M	396	SER
1	M	404	GLU
1	M	408	THR
1	M	412	ARG
1	M	424	LEU
1	M	428	LEU
1	N	1	MSE
1	N	6	LEU
1	N	10	LEU
1	N	26	THR
1	N	34	SER

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Mol	Chain	Res	Type
1	N	36	GLN
1	N	41	LYS
1	N	45	THR
1	N	52	HIS
1	N	54	LEU
1	N	76	LEU
1	N	77	LYS
1	N	79	VAL
1	N	82	LEU
1	N	85	LEU
1	N	103	ASN
1	N	115	LEU
1	N	119	LEU
1	N	123	LEU
1	N	143	THR
1	N	148	VAL
1	N	154	LYS
1	N	184	ILE
1	N	191	SER
1	N	201	PRO
1	N	212	VAL
1	N	215	ILE
1	N	221	ARG
1	N	233	LEU
1	N	242	THR
1	N	248	SER
1	N	251	LEU
1	N	254	ILE
1	N	255	LEU
1	N	257	ILE
1	N	258	LEU
1	N	259	SER
1	N	265	LEU
1	N	266	ASP
1	N	267	ASP
1	N	268	SER
1	N	269	LEU
1	N	286	SER
1	N	290	SER
1	N	291	SER
1	N	304	MSE
1	N	337	LEU

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Mol	Chain	Res	Type
1	N	363	LEU
1	N	380	LEU
1	N	391	ARG
1	N	404	GLU
1	N	414	THR
1	N	419	ILE
1	N	424	LEU
1	N	428	LEU
1	O	1	MSE
1	O	3	LEU
1	O	6	LEU
1	O	10	LEU
1	O	27	GLU
1	O	29	ILE
1	O	33	GLU
1	O	45	THR
1	O	54	LEU
1	O	60	LYS
1	O	64	ASN
1	O	66	THR
1	O	76	LEU
1	O	78	THR
1	O	82	LEU
1	O	85	LEU
1	O	108	LEU
1	O	115	LEU
1	O	117	SER
1	O	119	LEU
1	O	122	ILE
1	O	123	LEU
1	O	129	ASP
1	O	134	ASP
1	O	146	ARG
1	O	154	LYS
1	O	176	VAL
1	O	184	ILE
1	O	192	SER
1	O	196	HIS
1	O	205	ILE
1	O	212	VAL
1	O	215	ILE
1	O	221	ARG

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Mol	Chain	Res	Type
1	O	226	PRO
1	O	242	THR
1	O	251	LEU
1	O	252	SER
1	O	254	ILE
1	O	255	LEU
1	O	258	LEU
1	O	265	LEU
1	O	269	LEU
1	O	291	SER
1	O	304	MSE
1	O	337	LEU
1	O	340	SER
1	O	341	GLN
1	O	357	PHE
1	O	363	LEU
1	O	366	SER
1	O	375	SER
1	O	379	GLU
1	O	382	SER
1	O	391	ARG
1	O	396	SER
1	O	404	GLU
1	O	408	THR
1	O	414	THR
1	O	416	LEU
1	O	417	ASP
1	O	418	SER
1	O	424	LEU
1	O	428	LEU
1	P	1	MSE
1	P	26	THR
1	P	29	ILE
1	P	35	TYR
1	P	36	GLN
1	P	37	GLN
1	P	46	ASN
1	P	48	GLN
1	P	54	LEU
1	P	57	ILE
1	P	60	LYS
1	P	64	ASN

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Mol	Chain	Res	Type
1	P	66	THR
1	P	76	LEU
1	P	82	LEU
1	P	83	LEU
1	P	90	VAL
1	P	107	GLN
1	P	108	LEU
1	P	113	SER
1	P	115	LEU
1	P	117	SER
1	P	119	LEU
1	P	123	LEU
1	P	134	ASP
1	P	154	LYS
1	P	184	ILE
1	P	191	SER
1	P	192	SER
1	P	196	HIS
1	P	205	ILE
1	P	217	ARG
1	P	221	ARG
1	P	233	LEU
1	P	242	THR
1	P	251	LEU
1	P	254	ILE
1	P	255	LEU
1	P	258	LEU
1	P	259	SER
1	P	265	LEU
1	P	269	LEU
1	P	282	ILE
1	P	290	SER
1	P	292	THR
1	P	302	ASP
1	P	304	MSE
1	P	337	LEU
1	P	341	GLN
1	P	355	LEU
1	P	363	LEU
1	P	366	SER
1	P	379	GLU
1	P	386	ASP

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Mol	Chain	Res	Type
1	P	404	GLU
1	P	414	THR
1	P	416	LEU
1	P	424	LEU
1	P	428	LEU
1	Q	3	LEU
1	Q	4	GLN
1	Q	10	LEU
1	Q	26	THR
1	Q	35	TYR
1	Q	48	GLN
1	Q	52	HIS
1	Q	54	LEU
1	Q	60	LYS
1	Q	61	THR
1	Q	65	ASN
1	Q	76	LEU
1	Q	79	VAL
1	Q	108	LEU
1	Q	115	LEU
1	Q	119	LEU
1	Q	123	LEU
1	Q	128	GLU
1	Q	129	ASP
1	Q	176	VAL
1	Q	180	VAL
1	Q	192	SER
1	Q	196	HIS
1	Q	216	ARG
1	Q	221	ARG
1	Q	232	ASP
1	Q	233	LEU
1	Q	242	THR
1	Q	245	ILE
1	Q	248	SER
1	Q	251	LEU
1	Q	254	ILE
1	Q	255	LEU
1	Q	257	ILE
1	Q	259	SER
1	Q	265	LEU
1	Q	266	ASP

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Mol	Chain	Res	Type
1	Q	268	SER
1	Q	269	LEU
1	Q	277	LEU
1	Q	291	SER
1	Q	302	ASP
1	Q	304	MSE
1	Q	337	LEU
1	Q	341	GLN
1	Q	363	LEU
1	Q	379	GLU
1	Q	391	ARG
1	Q	396	SER
1	Q	404	GLU
1	Q	414	THR
1	Q	416	LEU
1	Q	417	ASP
1	Q	419	ILE
1	Q	424	LEU
1	Q	427	SER
1	Q	428	LEU
1	R	1	MSE
1	R	3	LEU
1	R	5	SER
1	R	13	VAL
1	R	26	THR
1	R	45	THR
1	R	54	LEU
1	R	56	GLU
1	R	60	LYS
1	R	61	THR
1	R	66	THR
1	R	76	LEU
1	R	82	LEU
1	R	106	THR
1	R	115	LEU
1	R	119	LEU
1	R	123	LEU
1	R	129	ASP
1	R	154	LYS
1	R	191	SER
1	R	192	SER
1	R	196	HIS

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Mol	Chain	Res	Type
1	R	212	VAL
1	R	221	ARG
1	R	242	THR
1	R	251	LEU
1	R	254	ILE
1	R	255	LEU
1	R	257	ILE
1	R	264	SER
1	R	267	ASP
1	R	269	LEU
1	R	277	LEU
1	R	280	SER
1	R	304	MSE
1	R	340	SER
1	R	363	LEU
1	R	396	SER
1	R	404	GLU
1	R	416	LEU
1	R	428	LEU
1	S	10	LEU
1	S	26	THR
1	S	45	THR
1	S	52	HIS
1	S	54	LEU
1	S	55	ASP
1	S	57	ILE
1	S	60	LYS
1	S	65	ASN
1	S	66	THR
1	S	76	LEU
1	S	77	LYS
1	S	82	LEU
1	S	87	ARG
1	S	90	VAL
1	S	115	LEU
1	S	119	LEU
1	S	123	LEU
1	S	149	ASP
1	S	156	ILE
1	S	176	VAL
1	S	180	VAL
1	S	196	HIS

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Mol	Chain	Res	Type
1	S	210	VAL
1	S	221	ARG
1	S	233	LEU
1	S	242	THR
1	S	251	LEU
1	S	254	ILE
1	S	255	LEU
1	S	257	ILE
1	S	258	LEU
1	S	265	LEU
1	S	267	ASP
1	S	268	SER
1	S	269	LEU
1	S	277	LEU
1	S	304	MSE
1	S	337	LEU
1	S	383	THR
1	S	404	GLU
1	S	414	THR
1	S	424	LEU
1	S	427	SER
1	S	428	LEU
1	T	27	GLU
1	T	36	GLN
1	T	41	LYS
1	T	45	THR
1	T	55	ASP
1	T	57	ILE
1	T	61	THR
1	T	76	LEU
1	T	78	THR
1	T	82	LEU
1	T	85	LEU
1	T	90	VAL
1	T	104	SER
1	T	108	LEU
1	T	113	SER
1	T	115	LEU
1	T	119	LEU
1	T	134	ASP
1	T	143	THR
1	T	149	ASP

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Mol	Chain	Res	Type
1	T	156	ILE
1	T	191	SER
1	T	196	HIS
1	T	221	ARG
1	T	242	THR
1	T	251	LEU
1	T	255	LEU
1	T	257	ILE
1	T	258	LEU
1	T	259	SER
1	T	265	LEU
1	T	266	ASP
1	T	267	ASP
1	T	269	LEU
1	T	286	SER
1	T	291	SER
1	T	304	MSE
1	T	337	LEU
1	T	341	GLN
1	T	362	LYS
1	T	363	LEU
1	T	372	ILE
1	T	383	THR
1	T	396	SER
1	T	400	LYS
1	T	404	GLU
1	T	415	ARG
1	T	421	VAL
1	T	424	LEU
1	T	428	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	ASN
1	A	165	GLN
1	A	170	GLN
1	A	200	ASN
1	A	368	HIS
1	A	378	GLN
1	B	12	ASN
1	B	65	ASN

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Mol	Chain	Res	Type
1	B	301	HIS
1	C	36	GLN
1	E	96	GLN
1	E	103	ASN
1	E	185	GLN
1	F	46	ASN
1	F	185	GLN
1	F	353	ASN
1	F	368	HIS
1	G	42	GLN
1	G	52	HIS
1	G	103	ASN
1	G	170	GLN
1	G	196	HIS
1	H	107	GLN
1	I	43	ASN
1	I	103	ASN
1	I	107	GLN
1	I	196	HIS
1	I	197	HIS
1	J	36	GLN
1	J	107	GLN
1	J	200	ASN
1	J	353	ASN
1	K	103	ASN
1	K	260	HIS
1	K	353	ASN
1	K	395	HIS
1	L	170	GLN
1	L	185	GLN
1	L	196	HIS
1	L	368	HIS
1	M	36	GLN
1	M	103	ASN
1	M	107	GLN
1	M	126	HIS
1	M	185	GLN
1	M	260	HIS
1	M	368	HIS
1	N	36	GLN
1	N	96	GLN
1	N	107	GLN

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Mol	Chain	Res	Type
1	N	126	HIS
1	N	185	GLN
1	N	227	GLN
1	O	42	GLN
1	O	65	ASN
1	O	107	GLN
1	O	170	GLN
1	O	301	HIS
1	P	48	GLN
1	P	96	GLN
1	P	107	GLN
1	P	341	GLN
1	P	426	ASN
1	Q	36	GLN
1	Q	37	GLN
1	Q	42	GLN
1	Q	48	GLN
1	Q	197	HIS
1	R	4	GLN
1	R	36	GLN
1	R	107	GLN
1	R	301	HIS
1	R	368	HIS
1	S	36	GLN
1	S	42	GLN
1	S	48	GLN
1	S	107	GLN
1	S	197	HIS
1	S	200	ASN
1	S	353	ASN
1	T	15	HIS
1	T	36	GLN
1	T	48	GLN
1	T	107	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	397/434 (91%)	-0.49	0 100 100	56, 93, 146, 184	0
1	B	386/434 (88%)	-0.48	2 (0%) 87 76	55, 89, 133, 176	0
1	C	386/434 (88%)	-0.60	1 (0%) 90 82	56, 80, 125, 155	0
1	D	386/434 (88%)	-0.50	1 (0%) 90 82	56, 86, 126, 166	0
1	E	386/434 (88%)	-0.53	3 (0%) 82 68	55, 86, 144, 192	0
1	F	386/434 (88%)	-0.52	2 (0%) 87 76	57, 93, 130, 164	0
1	G	386/434 (88%)	-0.54	1 (0%) 90 82	53, 84, 123, 149	0
1	H	386/434 (88%)	-0.38	1 (0%) 90 82	56, 102, 155, 199	0
1	I	386/434 (88%)	-0.53	0 100 100	51, 85, 124, 171	0
1	J	386/434 (88%)	-0.50	1 (0%) 90 82	52, 93, 137, 179	0
1	K	397/434 (91%)	-0.51	2 (0%) 87 76	58, 89, 139, 212	0
1	L	386/434 (88%)	-0.56	1 (0%) 90 82	51, 84, 126, 168	0
1	M	386/434 (88%)	-0.49	1 (0%) 90 82	48, 85, 144, 176	0
1	N	386/434 (88%)	-0.51	2 (0%) 87 76	50, 85, 133, 177	0
1	O	386/434 (88%)	-0.60	1 (0%) 90 82	47, 77, 117, 162	0
1	P	386/434 (88%)	-0.54	2 (0%) 87 76	53, 85, 142, 188	0
1	Q	386/434 (88%)	-0.43	3 (0%) 82 68	51, 101, 154, 201	0
1	R	386/434 (88%)	-0.60	1 (0%) 90 82	54, 85, 129, 164	0
1	S	386/434 (88%)	-0.41	1 (0%) 90 82	69, 106, 155, 189	0
1	T	386/434 (88%)	-0.49	1 (0%) 90 82	62, 94, 151, 193	0
All	All	7742/8680 (89%)	-0.51	27 (0%) 90 82	47, 89, 141, 212	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	161	ASP	3.4
1	Q	164	SER	2.9
1	E	24	ASP	2.8
1	F	305	SER	2.6
1	E	164	SER	2.5
1	K	16	GLU	2.5
1	N	24	ASP	2.5
1	B	262	CYS	2.5
1	G	164	SER	2.5
1	N	164	SER	2.4
1	L	431	VAL	2.4
1	E	262	CYS	2.3
1	Q	165	GLN	2.3
1	K	330	GLN	2.3
1	D	24	ASP	2.3
1	M	15	HIS	2.2
1	F	161	ASP	2.2
1	J	161	ASP	2.2
1	T	3	LEU	2.1
1	Q	160	GLY	2.1
1	H	262	CYS	2.1
1	C	305	SER	2.1
1	R	336	SER	2.1
1	S	336	SER	2.1
1	B	56	GLU	2.1
1	P	336	SER	2.0
1	P	2	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.